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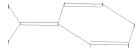
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chain nodes:
7 8 9
ring nodes:
1 2 3 4 5 6
chain bonds:
2-7 7-8 7-9
ring bonds:
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds:
1-2 1-6 2-3 3-4 4-5 5-6
exact bonds:
2-7 7-8 7-9
isolated ring systems:
containing 1:

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS

L1 STRUCTURE UPLOADED

=> d 11 L1 HAS NO ANSWERS L1 STR

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=> s 11 sss sam SAMPLE SEARCH INITIATED 15:19:14 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 221 TO ITERATE

100.0% PROCESSED 221 ITERATIONS SEARCH TIME: 00.00.01 14 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
PROJECTED ITERATIONS: 3529 TO 5311
PROJECTED ANSWERS: 56 TO 504

L2 14 SEA SSS SAM L1

=> s 11 sss full FULL SEARCH INITIATED 15:19:22 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 4999 TO ITERATE

100.0% PROCESSED 4999 ITERATIONS 233 ANSWERS SEARCH TIME: 00.00.01

L3 233 SEA SSS FUL L1

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 TOTAL

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(The Retro-Diels-Alder Reaction Part II. Dienophiles with One or More

Heteroatom)

RN 54133-10-7 CAPLUS

CN Propanedinitrile, 2-(1-methyl-2,3,5,6-tetraphenyl-4(1H)-pyridinylidene)-(CA INDEX NAME)

ANSWER 2 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2007:171924 CAPLUS

DOCUMENT NUMBER: 146:258239

TITLE: Use of ionic 1.4-dihydropyridine UV-A sunscreens INVENTOR(S): Berg-Schultz, Katja; Mendrok-Edinger, Christine; Poschalko, Alexander; Westenfelder, Horst

PATENT ASSIGNEE(S): DSM IP Assets B.V., Neth.

SOURCE: PCT Int. Appl., 92pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO. | | | | | KIND | | DATE | | APPLICATION NO. | | | | | | | | | |
|------------|------|-----|------|-----|------|-----|------|------|-----------------|------|-----|------|-----|-----|------------|------|-------|--|
| | 2007 | | | | A1 | _ | 2007 | 0215 | WO 2006-EP7691 | | | | | | 20060803 < | | | |
| | W: | ΑE, | AG, | AL, | AM, | AT, | AU, | AZ, | BA, | BB, | BG, | BR, | BW, | BY, | BZ, | CA, | CH, | |
| | | CN, | co, | CR, | CU, | CZ, | DE, | DK, | DM, | DZ, | EC, | EE, | EG, | ES, | FI, | GB, | GD, | |
| | | GE, | GH, | GM, | HN, | HR, | HU, | ID, | IL, | IN, | IS, | JP, | KE, | KG, | KM, | KN, | KP, | |
| | | KR, | ΚZ, | LA, | LC, | LK, | LR, | LS, | LT, | LU, | LV, | LY, | MA, | MD, | MG, | MK, | MN, | |
| | | MW, | MX, | MZ, | NA, | NG, | NI, | NO, | NZ, | OM, | PG, | PH, | PL, | PT, | RO, | RS, | RU, | |
| | | SC, | SD, | SE, | SG, | SK, | SL, | SM, | SY, | ΤJ, | TM, | TN, | TR, | TT, | TZ, | UA, | UG, | |
| | | US, | UZ, | VC, | VN, | ZA, | ZM, | ZW | | | | | | | | | | |
| | RW: | ΑT, | BE, | BG, | CH, | CY, | CZ, | DE, | DK, | EE, | ES, | FI, | FR, | GB, | GR, | HU, | IE, | |
| | | IS, | IT, | LT, | LU, | LV, | MC, | NL, | PL, | PT, | RO, | SE, | SI, | SK, | TR, | BF, | BJ, | |
| | | CF, | CG, | CI, | CM, | GA, | GN, | GQ, | GW, | ML, | MR, | NE, | SN, | TD, | TG, | BW, | GH, | |
| | | GM, | KE, | LS, | MW, | ΜZ, | NA, | SD, | SL, | SZ, | TZ, | UG, | ZM, | ZW, | AM, | ΑZ, | BY, | |
| | | KG, | ΚZ, | MD, | RU, | ТJ, | TM | | | | | | | | | | | |
| TTL | 700 | TAT | TNEO | | | | | | | PD 2 | 005 | 1704 | 1 | | 2 2 | 0050 | 205 / | |

PRIORITY APPLN. INFO.: EP 2005-17041

OTHER SOURCE(S):

AΒ The present invention relates to advantageous uses of 1,4-dihydropyridine derivs, and to novel cosmetic or dermatol, sunscreen compns, containing

1,4-dihydropyridine derivs. Thus,

4-dicyanomethylene-2,6-dimethyl-1,4-dihydropyridine-N-

MARPAT 146:258239

(ethyloxyethyloxyphosphate ester monosodium salt) was prepared and formulated at 2% together with 4% Parsol MCX into an oil/water sunscreen lotion which absorbs in the UV-A and UV-B range.

863406-54-6P 863406-56-8P 863406-58-0P 863406-60-4P 863406-62-6P 863406-63-7P 863406-64-8P 863406-65-9P 863406-66-0P 863406-67-1P 863406-68-2P 863406-69-3P 863406-70-6P 863406-72-8P 863406-73-9P

| 863 | 406-74-0P | 863406-75-1P | 863406-76-2P |
|-----|-----------|--------------|--------------|
| 863 | 406-77-3P | 863406-78-4P | 863406-79-5P |
| 863 | 406-80-8P | 863406-81-9P | 863406-99-9P |
| 863 | 407-00-5P | 863407-01-6P | 863407-02-7P |
| 863 | 407-03-8P | 924726-36-3P | 924726-37-4P |
| 924 | 726-38-5P | 924726-39-6P | 924726-40-9P |
| 924 | 726-42-1D | | |

924726-42-1P RL: COS (Cosmetic use); SPN (Synthetic preparation); THU (Therapeutic

use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation and compns. of ionic 1,4-dihydropyridine UV-A cosmetic or

(preparation and compns. of ionic 1,4-dihydropyridine UV-A cosmetic or dermatol. sunscreens)

RN 863406-54-6 CAPLUS

CN Propanedinitrile, 2-[2,6-dimethyl-1-[2-[2-(phosphonooxy)ethoxy]ethyl]-4(1H)-pyridinylidene]-, sodium salt (1:1) (CA INDEX NAME)

Na

RN 863406-56-8 CAPLUS

CN Propanedinitrile, 2-[2,6-dimethyl-1-[2-(sulfooxy)ethyl]-4(1H)pyridinylidene]-, sodium salt (1:1) (CA INDEX NAME)

Na

RN 863406-58-0 CAPLUS CN 1(4H)-Pyridinepropa:

 $\label{localization} $$1(4H)-Pyridine propanaminium, 4-(dicyanomethylene)-N-[2-(2-hydroxyethoxy)ethyl]-N,N,2,6-tetramethyl-, iodide (1:1) (CA INDEX NAME)$

$$\begin{array}{c} \text{Me} \\ \text{(CH2)} \ 3 - \text{N}^{\frac{1}{2}} \ \text{CH}_2 - \text{CH}_2 - \text{O} - \text{CH}_2 - \text{CH}_2 - \text{OH} \\ \text{NC} - \text{C} \\ \text{NMe} \\ \text{CN} \end{array}$$

• ı-

RN 863406-60-4 CAPLUS
CN Pyridinium, 1-[2-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)pyridinyl]ethoxy[ethyl]-, chloride (1:1) (CA INDEX NAME)

● C1-

RN 863406-62-6 CAPLUS
CN 1-Propanesulfonic acid, 3-[3-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)-pyridinyl]phenoxyl-, sodium salt (1:1) (CA INDEX NAME)

Na

RN 863406-63-7 CAPLUS
CN Propanedintrile, 2-[2,6-dimethyl-1-[2-(sulfooxy)ethyl]-4(1H)pyridinylidene]-, potassium salt (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{CH}_2\text{--}\text{CH}_2\text{--}\text{OSO}_3\text{H} \\ \text{NC--} \\ \text{CN} \end{array}$$

• •

RN 863406-64-8 CAPLUS

CN 1(4H)-Pyridinepropanaminium, 4-(dicyanomethylene)-N-[2-[2-(2-hydroxyethoxy]ethoxy]ethyl]-N,N,2,6-tetramethyl-, chloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} & \text{Me} \\ & \text{Me} \\ & \text{(CH}_2)_3 - \text{N}^{\frac{1}{2}} \text{ CH}_2 - \text{CH}_2 - \text{O} - \text{CH}_2 - \text{CH}_2 - \text{O} + \text{CH}_2 - \text{CH}_2 - \text{O} + \text{CH}_2 - \text{CH}_2 - \text{O} + \text{CH}_2 - \text{CH}_2$$

● C1-

RN 863406-65-9 CAPLUS

CN

1(4H)-Pyridinepropanaminium, 4-(dicyanomethylene)-N,N,N,2,6-pentamethyl-, iodide (1:1) (CA INDEX NAME)

• I-

RN 863406-66-0 CAPLUS

CN Pyridinium, 1-[2-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)-pyridinyl]ethyl]-, bromide (1:1) (CA INDEX NAME)

• Br-

RN 863406-67-1 CAPLUS

CN Phosphonic acid, P-[3-[2-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)-pyridinyl]ethoxy]propyl]-, sodium salt (1:1) (CA INDEX NAME)

Na

RN 863406-68-2 CAPLUS

CN 1(4H)-Pyridinepropanesulfonic acid, 4-(dicyanomethylene)-2,6-dimethyl-, potassium salt (1:1) (CA INDEX NAME)

K

RN 863406-69-3 CAPLUS

CN 1-Propanesulfonic acid, 3-[2-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)-pyridinyl]ethoxy]-, sodium salt (1:1) (CA INDEX NAME)

Na

RN 863406-70-6 CAPLUS

CN Phosphonic acid, P-[3-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)-pyridinyl]propyl]-, potassium salt (1:2) (CA INDEX NAME)

● 2 K

RN 863406-72-8 CAPLUS

CN 1(4H)-Pyridinebutanesulfonic acid, 4-(dicyanomethylene)-2,6-dimethyl-, compd. with 2,2',2''-nitrilotris[ethanol] (1:1) (CA INDEX NAME)

CM

CRN 863406-71-7

CMF C14 H17 N3 O3 S

CM

CRN 102-71-6 CMF C6 H15 N O3 CH2-CH2-ОН

HO-CH2-CH2-N-CH2-CH2-OH

RN 863406-73-9 CAPLUS

CN Propanedinitrile, [2,6-dimethyl-1-[2-(sulfooxy)ethyl]-4(IH)pyridinylidene]-, compd. with 2,2',2''-nitrilotris[ethanol] (1:1) (CA INDEX NAME)

CM 1

CRN 863406-55-7

CMF C12 H13 N3 O4 S

CM :

CRN 102-71-6 CMF C6 H15 N O3

СH2-СH2-ОН

HO-CH2-CH2-N-CH2-CH2-OH

RN 863406-74-0 CAPLUS

CN Benzenesulfonic acid, 4-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)-pyridinyl]-, sodium salt (1:1) (CA INDEX NAME)

Na

RN 863406-75-1 CAPLUS

CN Benzenesulfonic acid, 3-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)pyridinyl]-, potassium salt (1:1) (CA INDEX NAME)

● K

- RN 863406-76-2 CAPLUS
- CN 1,3-Benzenedisulfonic acid, 5-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)-pyridinyl]-, potassium salt (1:1) (CA INDEX NAME)

K

- RN 863406-77-3 CAPLUS
- CN Phosphonic acid, P-[3-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)pyridinyl]phenyl]-, lithium salt (1:1) (CA INDEX NAME)

• Li

- RN 863406-78-4 CAPLUS
- CN Propanedinitrile, 2-[1-[3-[bis[2-(sulfooxy)ethyl]amino]propyl]-2,6dimethyl-4(lH)-pyridinylidene]-, sodium salt (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{CH}_2-\text{CH}_2-\text{OSO}_3\text{H} \\ \text{CH}_2)_3-\text{N-CH}_2-\text{CH}_2-\text{OSO}_3\text{H} \\ \text{NC-C} \\ \text{Me} \\ \end{array}$$

Na

RN 863406-79-5 CAPLUS CN Propanedinitrile, 2-[2,6-dimethyl-1-[2-[2-[2-[2-(sulfooxy)ethoxy]ethoxy]ethoxy]ethoxy]ethyl]-4(1H)-pyridinylidene]-, potassium salt (1:1) (CA INDEX NAME)

K

- RN 863406-80-8 CAPLUS CN Propanedinitrile, 2-[2,6-bis(1,1-dimethylethyl)-1-[2-[2-
 - (phosphonooxy)ethoxy]ethyl]-4(1H)-pyridinylidene]-, sodium salt (1:1) (CA INDEX NAME)

Na

- RN 863406-81-9 CAPLUS
- Propanedinitrile, 2-[2,6-diethy1-3,5-dimethy1-1-[2-(sulfooxy)ethy1]-4(1H)-1-[2-(sulfCN pyridinylidene]-, potassium salt (1:1) (CA INDEX NAME)

K

RN 863406-99-9 CAPLUS

CN 1-Propanesulfonic acid, 3-[4-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)-pyridinyl]phenoxy]-, potassium salt (1:1) (CA INDEX NAME)

K

RN 863407-00-5 CAPLUS

Propanedinitrile, 2-[2,6-dimethyl-1-[2-(sulfooxy)ethyl]-4(1H)-pyridinylidene]-, compd. with 2-amino-2-methyl-1-propanol (1:1) (CA INDEX NAME)

CM 1

CN

CRN 863406-55-7 CMF C12 H13 N3 O4 S

CM 2

CRN 124-68-5 CMF C4 H11 N O

RN 863407-01-6 CAPLUS

CN 1(4H)-Pyridinepropanaminium, 4-(dicyanomethylene)-N,N,2,6-tetramethyl-N-(2-sulfoethyl)-, inner salt (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{(CH2)} \ 3 - \text{N} \\ \text{Me} \\ \text{NC} - \text{C} \\ \text{CN} \end{array}$$

RN 863407-02-7 CAPLUS

CN Guanidine, N-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)-pyridinyl]-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 863407-03-8 CAPLUS

CN

Guanidine, N-[2-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)-pyridinyl]ethyl]-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

- RN 924726-36-3 CAPLUS
- CN Propanedinitrile, 2-[2,6-dimethyl-1-[2-(sulfooxy)ethyl]-4(1H)pyridinylidene]-, ammonium salt (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{CH}_2-\text{CH}_2-\text{OSO}_3\text{H} \\ \text{NC}-\text{C} \\ \text{NMe} \\ \text{CN} \end{array}$$

- NH3
- RN 924726-37-4 CAPLUS
- CN Propanedinitrile, 2-[2,6-dimethyl-1-[2-(sulfooxy)ethyl]-4(1H)pyridinylidene]-, lithium salt (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{CH}_2-\text{CH}_2-\text{OSO}_3\text{H} \\ \text{NC}-\text{CN} \end{array}$$

- Li
- RN 924726-38-5 CAPLUS
- CN Propanedinitrile, 2-[2,6-dimethyl-1-[2-(sulfooxy)ethyl]-4(1H)pyridinylidene]-, magnesium salt (2:1) (CA INDEX NAME)

- ●1/2 Mg
- RN 924726-39-6 CAPLUS
- CN Propanedinitrile, 2-[2,6-dimethyl-1-[2-(sulfooxy)ethyl]-4(1H)pyridinylidene]-, calcium salt (2:1) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{CH}_2\text{--}\text{CH}_2\text{--}\text{OSO}_3\text{H} \\ \text{NC--} \\ \text{CN} \end{array}$$

●1/2 Ca

RN 924726-40-9 CAPLUS CN L-Aspartic acid, N-[3-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)pyridinyl]propyl]-, sodium salt (1:2) (CA INDEX NAME)

Absolute stereochemistry.

●2 Na

RN 924726-42-1 CAPLUS CN

1(4H)-Pyridinepropanesulfonic acid, 4-(dicyanomethylene)-2,6-dimethyl-, compd. with 2,2',2''-nitrilotris[ethanol] (1:1) (CA INDEX NAME)

CM

1

CRN 863477-45-6 CMF C13 H15 N3 O3 S

CM

CRN 102-71-6 CMF C6 H15 N O3

но- ch2- ch2- n- ch2- ch2- он

- IT 403830-93-3P 863406-52-4P 863406-57-9P 863406-59-1P 863406-61-5P
 - RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 - (preparation and compns. of ionic 1,4-dihydropyridine UV-A cosmetic or dermatol. sunscreens)
 N 403830-93-3 CAPLUS
- RN 403830-93-3 CAPLUS
 CN Propanedinitrile, 2-[1-(2-hydroxyethyl)-2,6-dimethyl-4(1H)-pyridinylidene](CA INDEX NAME)

- RN 863406-52-4 CAPLUS
- CN Propanedinitrile, 2-[1-[2-(2-hydroxyethoxy)ethy1]-2,6-dimethyl-4(1H)pyridinylidene|- (CA INDEX NAME)

- RN 863406-57-9 CAPLUS
- CN Propanedinitrile, 2-[1-[3-(dimethylamino)propyl]-2,6-dimethyl-4(1H)-pyridinylidene]- (CA INDEX NAME)

- RN 863406-59-1 CAPLUS
- CN Propanedinitrile, 2-[1-[2-(2-chloroethoxy)ethyl]-2,6-dimethyl-4(1H)-pyridinylidene]- (CA INDEX NAME)

RN 863406-61-5 CAPLUS

CN Propanedinitrile, 2-[1-(3-hydroxyphenyl)-2,6-dimethyl-4(1H)-pyridinylidene]- (CA INDEX NAME)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2005:1075592 CAPLUS

DOCUMENT NUMBER: 143:372818

TITLE: UV absorbing chromophores covalently bonded to hyperbranched polymers for sunscreens

INVENTOR(S): Poschalko, Alexander; Huber, Ulrich; Schehlmann,

Volker

PATENT ASSIGNEE(S): DSM Ip Assets B. V., Neth.

SOURCE: PCT Int. Appl., 60 pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

| PAT | TENT : | NO. | | | KIN | D | DATE | | | APPL | ICAT | ION : | NO. | | D | ATE | | |
|---------------|--------|-------|-----|-----|-------------|-----|------|----------------|-----|------|------|-------|-----|------------|-----|------|-------|----|
| WO 2005092282 | | | | | A1 20051006 | | | WO 2005-EP3117 | | | | | | 20050323 < | | | | |
| | W: | ΑE, | AG, | AL, | AM, | AT, | AU, | AZ, | BA, | BB, | BG, | BR, | BW, | BY, | BZ, | CA, | CH, | |
| | | CN, | CO, | CR, | CU, | CZ, | DE, | DK, | DM, | DZ, | EC, | EE, | EG, | ES, | FI, | GB, | GD, | |
| | | GE, | GH, | GM, | HR, | HU, | ID, | IL, | IN, | IS, | JP, | KE, | KG, | KP, | KR, | KZ, | LC, | |
| | | LK, | LR, | LS, | LT, | LU, | LV, | MA, | MD, | MG, | MK, | MN, | MW, | MX, | MZ, | NA, | NI, | |
| | | NO, | NZ, | OM, | PG, | PH, | PL, | PT, | RO, | RU, | SC, | SD, | SE, | SG, | SK, | SL, | SM, | |
| | | SY, | TJ, | TM, | TN, | TR, | TT, | TZ, | UA, | UG, | US, | UZ, | VC, | VN, | YU, | ZA, | ZM, | ZW |
| | RW: | BW, | GH, | GM, | KE, | LS, | MW, | MZ, | NA, | SD, | SL, | SZ, | TZ, | UG, | ZM, | ZW, | AM, | |
| | | ΑZ, | BY, | KG, | KΖ, | MD, | RU, | ΤJ, | TM, | ΑT, | BE, | ВG, | CH, | CY, | CZ, | DE, | DK, | |
| | | EE, | ES, | FI, | FR, | GB, | GR, | HU, | IE, | IS, | IT, | LT, | LU, | MC, | NL, | PL, | PT, | |
| | | RO, | SE, | SI, | SK, | TR, | BF, | ΒJ, | CF, | CG, | CI, | CM, | GA, | GN, | GQ, | GW, | ML, | |
| | | MR, | NE, | SN, | TD, | TG | | | | | | | | | | | | |
| ΑU | 2005 | 2269: | 22 | | A1 | | 2005 | 1006 | | AU 2 | 005- | 2269 | 22 | | 2 | 0050 | 323 - | < |
| ΑU | 2005 | 2269: | 22 | | B2 | | 2010 | 0304 | | | | | | | | | | |
| EP | 1727 | 515 | | | A1 | | 2006 | 1206 | | EP 2 | 005- | 7163 | 37 | | 2 | 0050 | 323 - | < |
| | R: | AT, | BE, | BG, | CH, | CY, | CZ, | DE, | DK, | EE, | ES, | FI, | FR, | GB, | GR, | HU, | IE, | |

IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR CN 1937999 Α 20070328 CN 2005-80009487 20050323 <--JP 2007535588 Т 20071206 JP 2007-504356 20050323 <--IN 2006DN05063 20070713 IN 2006-DN5063 20060901 <--Α KR 2007001199 Α 20070103 KR 2006-719628 20060922 <--US 20080081025 A1 20080403 US 2006-593486 20061017 <--PRIORITY APPLN. INFO .: EP 2004-7201 20040325 <--WO 2005-EP3117 20050323 <--

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

The invention provides a conjugate comprising a hyperbranched polymer covalently bonded to at least three UV absorbing chromophores having an UV absorption maximum \$\text{\text{Max}} \text{ } \text{270 nm.}\$ The conjugate is an effective and safe sunscreen which can advantageously be used in cosmetic compns. For example, poly(glycerol-b-propylene oxide) (5.0 g, 4.6 mmol) to afford 7.5 g mesylated poly(glycerol-b-propylene oxide). A polymeric UV filter was obtained by attaching 8.9 g of 4-(1.3-benzoxazol-2-yl)phenol to 7.48 g of the mesylated polymer to yield 4.82 g of the hyperbranched polymer chromophore with the theor. Chromophore content of 64%. A composition was prepared by mixing the hyperbranched polymer chromophore b.0 g, Brij 72 2.0 g. Brit 172 12.0 g. Lanette O 2.0 g. Brid GM 3650 2.0 g. BH 10.05 g, and Phenonip 0.8 g at 80°, adding a preheated solution of glycerin 4.0 g and EDTA BD 0.1 g in water 62.95 g, and subsequently 10% aqueous KOH 0.1 g as well as Sepigel 305 1.0 g. An average SPF was 6.6, compared to 6.8 of Parsol

IT 403830-93-3DP, reaction products with glycerol-propylene oxide block polymers

RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(UV absorbing chromophores covalently bonded to hyperbranched polymers for sunscreens)

403830-93-3 CAPLUS

CN Propanedinitrile, 2-[1-(2-hydroxyethyl)-2,6-dimethyl-4(1H)-pyridinylidene]-(CA INDEX NAME)

IT 403830-93-3P

RN

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(UV absorbing chromophores covalently bonded to hyperbranched polymers

(UV absorbing chromophores covalently bonded to hyperbranched polymers for sunscreens)

RN 403830-93-3 CAPLUS

Propanedinitrile, 2-[1-(2-hydroxyethy1)-2,6-dimethy1-4(1H)-pyridinylidene]-(CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{CH}_2\text{--}\text{CH}_2\text{--}\text{OH} \\ \\ \text{NC--} \\ \text{CN} \end{array}$$

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2005:962216 CAPLUS

DOCUMENT NUMBER: 143.253492

TITLE: Preparation of ionic UVA sunscreens

Patent

INVENTOR(S): Berg-Schultz, Katja; Huber, Ulrich; Sprenger, Daniel

PATENT ASSIGNEE(S): DSM Ip Assets B. V., Neth. PCT Int. Appl., 52 pp. SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE: LANGUAGE:

English FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| | | | | | | KIND DATE | | | | APPLICATION NO. | | | | | | | | | |
|-----------|----------|--------|---------|-------|------|-------------|------|--------|----------------|-----------------|------|------|------|------|------------|------|-----|---|--|
| WO | | | | | | 31 20050901 | | | WO 2005-EP1379 | | | | | | 20050211 < | | | | |
| | W: | | | | | | | | | | | BR, | | | | | | | |
| | | | | | | | | | | | | EE, | | | | | | | |
| | | | | | | | | | | | | KE, | | | | | | | |
| | | | | | | | | | | | | MN, | | | | | | | |
| | | | | | | | | | | | | SD, | | | | | | | |
| | | | | | | | | | | | | VC, | | | | | | | |
| | RW: | | | | | | | | | | | SZ, | | | | | | | |
| | | | | | | | | | | | | BG, | | | | | | | |
| | | | | | | | | | | | | LT, | | | | | | | |
| | | | | | | | | | | | | CM, | | | | | | | |
| | | | NE, | | | | , | 20, | 02/ | 00, | 01/ | 011/ | 011, | 0117 | 02/ | On y | , | | |
| IIA | 2005 | | | | | | 2005 | 0901 | | AII 2 | 005- | 2158 | 81 | | 2 | 0050 | 211 | < | |
| | 1716 | | | | | | | | | | | | | | | | | | |
| | | | | | | | | | | | | LI, | | | | | | | |
| | | | | | | | | | | | | HU, | | | | 1107 | , | | |
| CN | 1918 | | | | | | | | | | | | | | | 0050 | 211 | < | |
| | 2007 | | | | | | | | | | | | | | | | | | |
| TN | 2006 | CMU 2 | 915 | | ā | | 2007 | 0608 | | TM 2 | 006- | CM29 | 15 | | 2 | 0050 | 209 | 2 | |
| | 2006 | | | | | | | | | | | | | | | | | | |
| | 2007 | | | | | | | | | | | 5890 | | | | | | | |
| PRIORITY | | | | | AI | | 2007 | 1125 | | | | 3294 | | | | | | | |
| LILIONII | | D | 111E () | | | | | | | | | EP13 | | | | 0050 | | | |
| 3 COTONIC | DATE: 11 | T 0 TO | DIZ E | OD 11 | 0 03 | mmarm. | 2112 | TT 3 D | | | | | | | | 0000 | | | |

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT MARPAT 143:253492 OTHER SOURCE(S):

The present invention relates to novel 1,4-dihydropyridine derivs., to novel cosmetic or dermatol. sunscreen compns. containing these derivs. and the use of these derivs. for photoprotecting human skin and/or hair against UV radiation, in particular solar radiation. Thus, a

4-dicaynomethylene-2,6-dimethyl-1,4-dihydropyridine-N(ethoxysulfate ester monosodium salt) was prepared in a series of steps starting from

4-dicyanomethylene-4H-pyran. The above product (3%) was used to form a sunscreen formulation.

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863406-63-7
                     863406-64-8
                                      863406-65-9
     863406-66-0
                     863406-67-1
                                      863406-68-2
     863406-69-3
                     863406-70-6
                                      863406-72-8
     863406-73-9
                     863406-74-0
                                      863406-75-1
     863406-76-2
                     863406-77-3
                                      863406-78-4
     863406-79-5
                     863406-80-8
                                      863406-81-9
     863406-82-0
                     863406-99-9
                                      863407-00-5
     863407-01-6
                     863407-02-7
                                      863407-03-8
     RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
        (ionic UVA sunscreens and compons, containing them)
RN
     863406-63-7 CAPLUS
CN
    Propanedinitrile, 2-[2,6-dimethyl-1-[2-(sulfooxy)ethyl]-4(1H)-
     pyridinylidene]-, potassium salt (1:1) (CA INDEX NAME)
```

K

$$\begin{array}{c} \text{Me} & \text{Me} \\ \text{(CH}_2)_3 - \text{N}^{+} \text{CH}_2 - \text{CH}_2 - \text{O} - \text{CH}_2 - \text{CH}_2 - \text{O} + \text{CH}_2 - \text{CH}_2 - \text{OH}_2 \\ \text{NC} - \text{CN} & \text{Me} \\ \end{array}$$

● c1-

RN 863406-65-9 CAPLUS CN 1(4H)-Pyridinepropa

1(4H)-Pyridinepropanaminium, 4-(dicyanomethylene)-N,N,N,2,6-pentamethyl-, iodide (1:1) (CA INDEX NAME)

• I-

- RN 863406-66-0 CAPLUS
- CN Pyridinium, 1-[2-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)-pyridinyl]ethyl], bromide (1:1) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \\ \text{NC-CH}_2\text{-CH}_2^{-\frac{1}{2}}\text{N} \\ \text{NC-CN} & \\ \end{array}$$

• Br-

- RN 863406-67-1 CAPLUS
- CN Phosphonic acid, P-[3-[2-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)-pyridinyl]ethoxy]propyl]-, sodium salt (1:1) (CA INDEX NAME)

Na

- RN 863406-68-2 CAPLUS
- CN 1(4H)-Pyridinepropanesulfonic acid, 4-(dicyanomethylene)-2,6-dimethyl-, potassium salt (1:1) (CA INDEX NAME)

● K

- RN 863406-69-3 CAPLUS
- CN 1-Propanesulfonic acid, 3-[2-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)-pyridinyl]ethoxy]-, sodium salt (1:1) (CA INDEX NAME)

Na

- RN 863406-70-6 CAPLUS
- CN Phosphonic acid, P-[3-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)-pyridinyl]propyl]-, potassium salt (1:2) (CA INDEX NAME)

● 2 K

- RN 863406-72-8 CAPLUS
- CN 1(4H)-Pyridinebutanesulfonic acid, 4-(dicyanomethylene)-2,6-dimethyl-, compd. with 2,2',2''-nitrilotris[ethanol] (1:1) (CA INDEX NAME)

CM 1

- CRN 863406-71-7
- CMF C14 H17 N3 O3 S

CM 2

CRN 102-71-6 CMF C6 H15 N O3

CH2-CH2-ОН

HO-CH2-CH2-N-CH2-CH2-OH

RN 863406-73-9 CAPLUS

1

CN Propanedinitrile, [2,6-dimethyl-1-[2-(sulfooxy)ethyl]-4(1H)-pyridinylidene]-, compd. with 2,2',2''-nitrilotris[ethanol] (1:1) (CA INDEX NAME)

CM

CRN 863406-55-7 CMF C12 H13 N3 O4 S

CM 2

CRN 102-71-6 CMF C6 H15 N O3

СH2-СH2-ОН НО-СH2-СH2-N-СH2-СH2-ОН

RN 863406-74-0 CAPLUS
CN Benzensulfonic acid, 4-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)pyridinyl]-, sodium sait (1:1) (CA INDEX NAME)

• Na

- RN 863406-75-1 CAPLUS
- CN Benzenesulfonic acid, 3-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)-pyridinyl]-, potassium salt (1:1) (CA INDEX NAME)

K

- RN 863406-76-2 CAPLUS
- CN 1,3-Benzenedisulfonic acid, 5-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)-pyridinyl]-, potassium salt (1:1) (CA INDEX NAME)

K

- RN 863406-77-3 CAPLUS
- CN Phosphonic acid, P-[3-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)-pyridinyl]phenyl]-, lithium salt (1:1) (CA INDEX NAME)

• Li

- RN 863406-78-4 CAPLUS
- CN Propanedinitrile, 2-[1-[3-[bis[2-(sulfooxy)ethyl]amino]propyl]-2,6dimethyl-4(1H)-pyridinylidene]-, sodium salt (1:1) (CA INDEX NAME)

Na

- RN 863406-79-5 CAPLUS
- CN Propanedinitrile, 2-[2,6-dimethyl-1-[2-[2-[2-[2-(3uffooxy)ethoxy]e

K

- RN 863406-80-8 CAPLUS
- CN Propanedinitrile, 2-[2,6-bis(1,1-dimethylethyl)-1-[2-[2-(phosphonoxy)ethoxy]ethyl]-4(1H)-pyridinylidene]-, sodium salt (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{t-Bu} \\ \text{CH}_2\text{--}\text{CH}_2\text{--}\text{O--}\text{CH}_2\text{--}\text{CH}_2\text{--}\text{OPO}_3\text{H}_2 \\ \text{NC--} \\ \text{CN} \end{array}$$

■ NT=

RN 863406-81-9 CAPLUS

CN Propanedinitrile, 2-[2,6-diethyl-3,5-dimethyl-1-[2-(sulfooxy)ethyl]-4(1H)-pyridinylidene]-, potassium salt (1:1) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Et} & \text{CH}_2\text{--}\text{CH}_2\text{--}\text{OSO}_3\text{H} \\ \text{NC--} & \text{Et} & \text{Et} \\ \hline \text{CN} & \text{Me} \end{array}$$

K

RN 863406-82-0 CAPLUS

CN Aspartic acid, N-[3-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)pyridinyl]propyl]-, disodium salt (9CI) (CA INDEX NAME)

●2 Na

RN 863406-99-9 CAPLUS

1-Propanesulfonic acid, 3-[4-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)-pyridinyl]phenoxy]-, potassium salt (1:1) (CA INDEX NAME)

● K

RN 863407-00-5 CAPLUS

Propanedinitrile, 2-[2,6-dimethyl-1-[2-(sulfooxy)ethyl]-4(1H)pyridinylidene]-, compd. with 2-amino-2-methyl-1-propanol (1:1) (CA INDEX NAME)

CM 1

CN

CRN 863406-55-7

CMF C12 H13 N3 O4 S

CM 2

CRN 124-68-5 CMF C4 H11 N O

CN

RN 863407-01-6 CAPLUS

1(4H)-Pyridinepropanaminium, 4-(dicyanomethylene)-N,N,2,6-tetramethyl-N-(2-sulfoethyl)-, inner salt (CA INDEX NAME)

- RN 863407-02-7 CAPLUS
- CN Guanidine, N-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)-pyridinyl]-, hydrochloride (1:1) (CA INDEX NAME)

HC1

- RN 863407-03-8 CAPLUS
- CN Guanidine, N-[2-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)-pyridinyl]ethyl]-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{NC} \\ \text{CN} \end{array}$$

HC1

- IT 863406-54-6P 863406-56-8P 863406-58-0P 863406-60-4P 863406-62-6P RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (ionic UVA sunscreens and compans. containing them)
- RN 863406-54-6 CAPLUS
- CN Propanedinitrile, 2-[2,6-dimethy1-1-[2-[2-(phosphonooxy)ethoxy]ethy1]-4(1H)-pyridinylidene]-, sodium salt (1:1) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{CH}_2\text{--}\text{CH}_2\text{--}\text{O}\text{--}\text{CH}_2\text{--}\text{CH}_2\text{--}\text{OPO}_3\text{H}_2 \\ \text{NC}\text{--}\text{CN} \end{array}$$

Na

RN 863406-56-8 CAPLUS

CN Propanedinitrile, 2-[2,6-dimethyl-1-[2-(sulfooxy)ethyl]-4(1H)pyridinylidene]-, sodium salt (1:1) (CA INDEX NAME)

Na

RN 863406-58-0 CAPLUS CN 1(4H)-Pvridinepropa

1(4H)-Pyridinepropanaminium, 4-(dicyanomethylene)-N-[2-(2-hydroxyethoxy)ethyl]-N,N,2,6-tetramethyl-, iodide (1:1) (CA INDEX NAME)

• I-

RN 863406-60-4 CAPLUS

CN Pyridinium, 1-[2-[2-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)-pyridinyl]ethoxy]ethyl]-, chloride (1:1) (CA INDEX NAME)

• c1-

RN 863406-62-6 CAPLUS

CN 1-Propanesulfonic acid, 3-[3-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)-pyridinyl]phenoxy]-, sodium salt (1:1) (CA INDEX NAME)

Na

- IT 403830-93-3P 863406-52-4P 863406-53-5P 863406-55-7P 863406-57-9P 863406-59-1P
 - 863406-61-5P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 - (Reactant or reagent)
 (ionic UVA sunscreens and compns. containing them)
- RN 403830-93-3 CAPLUS
- CN Propanedinitrile, 2-[1-(2-hydroxyethyl)-2,6-dimethyl-4(1H)-pyridinylidene]-(CA INDEX NAME)

- RN 863406-52-4 CAPLUS
- CN Propanedinitrile, 2-[1-[2-(2-hydroxyethoxy)ethyl]-2,6-dimethyl-4(1H)pyridinylidene]- (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{CH}_2\text{-CH}_2\text{-O-CH}_2\text{-CH}_2\text{-OH} \\ \text{NC-C} \\ \text{Me} \\ \text{CN} \end{array}$$

- RN 863406-53-5 CAPLUS
- CN Phosphorodichloridic acid, 2-[2-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)-pyridinyl]ethoxy]ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} & \text{CH}_2\text{--}\text{CH}_2\text{--}\text{O}\text{--}\text{CH}_2\text{--}\text{CH}_2\text{--}\text{O}\text{--}\text{P-C} \\ \text{NC}\text{--} & \text{CN} \\ \end{array}$$

- RN 863406-55-7 CAPLUS
- CN Propanedinitrile, 2-[2,6-dimethyl-1-[2-(sulfooxy)ethyl]-4(1H)pyridinylidene]- (CA INDEX NAME)

- RN 863406-57-9 CAPLUS
- CN Propanedinitrile, 2-[1-[3-(dimethylamino)propyl]-2,6-dimethyl-4(1H)pyridinylidene]- (CA INDEX NAME)

- RN 863406-59-1 CAPLUS
- CN Propanedinitrile, 2-[1-[2-(2-chloroethoxy)ethyl]-2,6-dimethyl-4(1H)-pyridinylidene]- (CA INDEX NAME)

863406-61-5 CAPLUS CN Propanedinitrile, 2-[1-(3-hydroxyphenyl)-2,6-dimethyl-4(1H)pyridinylidenel- (CA INDEX NAME)

OS.CITING REF COUNT: THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD 1 (1 CITINGS)

REFERENCE COUNT: THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2005:523247 CAPLUS DOCUMENT NUMBER: 143:65134

TITLE: Microcapsules with UV filter activity

INVENTOR(S): Berg-Schultz, Katja DSM IP Assets B. V., Neth. PATENT ASSIGNEE(S):

SOURCE: PCT Int. Appl., 51 pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| | TENT : | | | | KIN | D : | DATE | | 1 | APPL: | | | | | | ATE | | |
|----|--------|-----|-----|-----|-----|-----|------|------|-----|-------|------|------|------|-----|-----|------|-------|---|
| | 2005 | | | | A1 | _ | 2005 | | 1 | | 004- | | | | | 0041 | | < |
| | W: | ΑE, | AG, | AL, | AM, | AT, | AU, | AZ, | BA, | BB, | BG, | BR, | BW, | BY, | BZ, | CA, | CH, | |
| | | CN, | CO, | CR, | CU, | CZ, | DE, | DK, | DM, | DZ, | EC, | EE, | EG, | ES, | FI, | GB, | GD, | |
| | | GE, | GH, | GM, | HR, | HU, | ID, | IL, | IN, | IS, | JP, | KΕ, | KG, | KP, | KR, | ΚZ, | LC, | |
| | | LK, | LR, | LS, | LT, | LU, | LV, | MA, | MD, | MG, | MK, | MN, | MW, | MX, | ΜZ, | ΝA, | NI, | |
| | | NO, | NZ, | OM, | PG, | PH, | PL, | PT, | RO, | RU, | SC, | SD, | SE, | SG, | SK, | SL, | SY, | |
| | | | | | | | | | | | | | | | ZA, | | | |
| | RW: | BW, | GH, | GM, | KE, | LS, | MW, | ΜZ, | NΑ, | SD, | SL, | SZ, | TZ, | UG, | ZM, | ZW, | AM, | |
| | | | | | | | | | | | | | | | CZ, | | | |
| | | | | | | | | | | | | | | | NL, | | | |
| | | | | | | | BF, | ΒJ, | CF, | CG, | CI, | CM, | GA, | GN, | GQ, | GW, | ML, | |
| | | | | | TD, | | | | | | | | | | | | | |
| EP | 1722 | | | | | | | | | | | | | | | | 202 < | < |
| | R: | | | | | | | | | | | | | | GR, | HU, | IE, | |
| | | | | | | | MC, | | | | | | | | | | | |
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| JP 2007519617 | T | 20070719 | JP : | 2006-541904 | | 20041202 < |
|------------------------|----|----------|------|--------------|------|------------|
| IN 2006CN01952 | A | 20070608 | IN: | 2006-CN1952 | | 20060602 < |
| KR 2006124606 | A | 20061205 | KR : | 2006-711002 | | 20060605 < |
| US 20070190325 | A1 | 20070816 | US : | 2007-581511 | | 20070227 < |
| PRIORITY APPLN. INFO.: | | | EP : | 2003-27847 | A | 20031204 < |
| | | | MO. | 2004-EP13734 | Tell | 20041202 < |

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

The invention provides a process for producing microcapsules with UV filter activity, wherein at least one type of crosslinkable chromophore with UV-A and/or UV-B and/or UV-C filter activity and optionally at least one type of crosslinkable monomer which does not have UV-A and/or UV-B and/or UV-B and/or UV-G filter activity are subjected to a crosslinking reaction in the absence of non-crosslinkable chromophores with UV-A and/or UV-B and/or UV-C filter activity and microcapsules obtainable by this process. Thus, 2-(4-)2-(triethoxysliyl)prop-2-enyloxy)benzylidene]malonic acid di-Bt ester (I) was prepared by the treatment of

[[4-(2-propynyloxy)phenyl]methylene]propanedioic acid di-Et ester with triethoxysilane. Microcapsules were obtained from I and tetraethoxysilane. Sunscreens comprised I 10.00% in addition to the conventional sunscreen emulsion components.

IT 853933-45-6 853933-46-7

RL: COS (Cosmetic use); PEP (Physical, engineering or chemical process); PYP (Physical process); BIOL (Biological study); PROC (Process); USES (Uses)

(microcapsules with UV filter activity)

N 853933-45-6 CAPLUS

$$\begin{array}{c} \text{Me} \\ \text{CH}_2\text{-CH} = \text{CH}_2 \\ \text{NC} - \\ \text{CN} \end{array}$$

RN 853933-46-7 CAPLUS

CN Propanedinitrile, 2-[2,6-dimethyl-1-(2-propyn-1-yl)-4(1H)-pyridinylidene]-(CA INDEX NAME)

OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
(4 CITINGS)

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN ACCESSION NUMBER: 2005:295737 CAPLUS

DOCUMENT NUMBER: 143:26106

TITLE: Perchloro-2,5,8-triazaphenalenyl Radical

AUTHOR(S): Zheng, Shijun; Thompson, Joe D.; Tontcheva, Ana; Khan,

Saeed I.; Rubin, Yves

Department of Chemistry and Biochemistry, University CORPORATE SOURCE: of California, Los Angeles, CA, 90095-1569, USA

Organic Letters (2005), 7(9), 1861-1863 SOURCE:

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE:

English

OTHER SOURCE(S): CASREACT 143:26106

The unusually stable perchloro-2,5,8-triazaphenalenyl radical 1 and its AB twisted dechlorinated dimer 2 were synthesized and characterized by ESR spectroscopy and x-ray crystallog. The x-ray structure of dimer 2 shows that the double bond connecting the two triazaphenalene systems is strongly twisted. Dimer 2 has a dramatic color shift from the solid state to solution, which may be due to a change of the twisting angle between both states.

852627-67-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(perchloro-2,5,8-triazaphenalenyl radical)

12

RN 852627-67-9 CAPLUS CN

3,5-Pyridinedicarboxylic acid, 4-(dicyanomethylene)-1,4-dihydro-, 3,5-diethyl ester (CA INDEX NAME)

TT

RECORD (12 CITINGS)

REFERENCE COUNT: THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS 15 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 7 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2004:670087 CAPLUS

DOCUMENT NUMBER: 141:429236

TITLE: Atomistic molecular modeling of electric field poling

of nonlinear optical polymers

AUTHOR(S): Leahy, Megan R.; Hayden, L. Michael

CORPORATE SOURCE: Physics Department, University of Baltimore County,

Baltimore, MD, 21250, USA PMSE Preprints (2004), 91, 269-270

SOURCE: CODEN: PPMRA9; ISSN: 1550-6703 PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal; (computer optical disk)

LANGUAGE: English

Fully atomistic mol. modeling methods were used to examine the elec. field-induced alignment of nonlinear optical (NLO) chromophores, methylpyridinemalonitrile (DNVMP) and DPNA embedded in PMMA host.

induced polar order was determined by calculating the average of cos30, where 0 is the angle between the direction of the dipole moment of the chromophore and the direction of the applied elec. field. This order

parameter was compared to that predicted by a non-interacting rigid gas model and to a model allowing for corrections due to intermol. electrostatic interactions. The ordering of the chromophores was studied as a function of chromophore concentration, size, and dipole moment.

16344-72-2

RL: PRP (Properties)

(elec. field induced polar order of NLO chromophores in polymer dispersions vs. concentration and mol. size)

16344-72-2 CAPLUS RN

CN Propanedinitrile, 2-(1-methyl-4(1H)-pyridinylidene)- (CA INDEX NAME)



THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 8 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2003:656538 CAPLUS

DOCUMENT NUMBER: 139:202103

TITLE: Sunscreen compositions as well as dihydropyridines and

dihydropyranes INVENTOR(S): Berg-Schultz, Katja

PATENT ASSIGNEE(S): Roche Vitamins A.-G., Switz.

SOURCE: PCT Int. Appl., 37 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE . English

FAMILY ACC. NUM. COUNT: 1

| | TENT : | | | | KIN | | DATE | | | APPL | | | | | D | ATE | | |
|---------------|------------------------------|------|------|-----|-------|-----|--------------|------|-----|------|------|------|------|------|------|------|------|-----|
| WO 2003068183 | | | | | 2003 | | | | | | | | 2 | 0030 | 204 | < | | |
| | W: | AE. | AG. | AL. | AM. | AT. | AU, | AZ. | BA. | BB. | BG. | BR. | BY. | BZ. | CA. | CH. | CN. | |
| | | | | | | | DK. | | | | | | | | | | | |
| | | GM. | HR. | HU. | ID. | IL. | IN, | IS. | JP. | KE. | KG. | KP. | KR. | KZ. | LC. | LK. | LR. | |
| | | | | | | | MD, | | | | | | | | | | | |
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| | RW: | | | | | | MZ, | | | SZ. | TZ. | UG. | ZM. | ZW. | AM. | AZ. | BY. | |
| | | KG. | KZ. | MD. | RU. | TJ. | TM, | AT. | BE. | BG. | CH, | CY. | CZ. | DE. | DK. | EE. | ES, | |
| | | | | | | | IE, | | | | | | | | | | | |
| | | | | CG, | CI, | CM, | GA, | | | | | | | | | | | |
| CA | 2473 | 228 | | | A1 | | 2003 | 0821 | | CA 2 | 003- | 2473 | 228 | | 2 | 0030 | 204 | < |
| AU | 2003
2003
1474 | 2068 | 25 | | A1 | | 2003 | 0904 | | AU 2 | 003- | 2068 | 25 | | 2 | 0030 | 204 | < |
| AU | 2003 | 2068 | 25 | | B2 | | 2007 | 0920 | | | | | | | | | | |
| EP | 1474 | 098 | | | A1 | | 2004 | 1110 | | EP 2 | 003- | 7045 | 23 | | 2 | 0030 | 204 | < |
| EP | 1474 | 098 | | | B1 | | 2006 | 0802 | | | | | | | | | | |
| | R: | AT, | BE, | CH, | DE, | DK, | ES, | FR, | GB, | GR, | IT, | LI, | LU, | NL, | SE, | MC, | PT, | |
| | | IE, | SI, | LT, | LV, | FI, | RO, | MK, | CY, | AL, | TR, | BG, | CZ, | EE, | HU, | SK | | |
| BR | 2003 | 0073 | 35 | | A | | 2004
2005 | 1207 | | BR 2 | 003- | 7335 | | | 2 | 0030 | 204 | < |
| CN | 1630 | 504 | | | A | | 2005 | 0622 | | CN 2 | 003- | 8036 | 94 | | 2 | 0030 | 204 | < |
| CN | 1005
2005
3347
2269 | 6362 | 2 | | C | | 2009 | 1202 | | | | | | | | | | |
| JP | 2005 | 5184 | 25 | | T | | 2005 | | | JP 2 | 003- | 5673 | 67 | | 2 | 0030 | 204 | < |
| AT | 3347 | 24 | | | T | | 2006 | 0815 | | AT 2 | nn3_ | 7045 | 23 | | 2 | 0030 | 204 | < |
| ES | 2269 | 978 | | | Т3 | | 2007 | | | ES 2 | 003- | 7045 | 23 | | 2 | 0030 | | |
| IN | 2004 | CN01 | 768 | | A | | 2006 | | | IN 2 | 004- | CN17 | 68 | | 2 | 0040 | 806 | < |
| | 2292 | | | | A1 | | 2009 | | | | | | | | | | | |
| | 2005 | | 278 | | A1 | | 2005 | | | US 2 | 004- | 4945 | 00 | | 2 | 0040 | 917 | < |
| | 7611 | | | | B2 | | 2009 | 1103 | | | | | | | | | | |
| RIT | Y APP | LN. | INFO | . : | | | | | | EP 2 | | | | | | | | |
| | | | | | | | | | | WO 2 | | | | | | 0030 | 204 | < |
| | ENT H | | | | | | | | | N LS | US D | ISPL | AY F | ORMA | T | | | |
| | DURCE | | | | | | | | | | | | | | | | | |
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| | 4-dih | | | | | | | | | | | | | | | | | |
| ph | otopr | otec | ting | hum | an si | kin | and/ | or h | air | agai | nst | UV r | adia | tion | , in | par | ticu | ıla |

AB solar radiation, and the use of such 1,4-dihydropyridine and/or 1,4-dihydropyrane derivs. as UV-A screening agents, particularly in cosmetic and pharmaceutical compns. For example, 1-N-(2-ethylhexyl)-4-dicyanomethylene-2,6-dimethyl-1,4-dihydropyridine and

ethyl(2,6-dimethylpyran-4-ylidene)cyanoacetate were prepared and included in cosmetics as sunscreen agents. 582297-74-3P

IT 16344-75-5P 49810-95-9P 582297-75-4P 582297-76-5P 582297-77-6P

582297-79-8P

RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(sunscreens comprising dihydropyridines or dihydropyranes)

16344-75-5 CAPLUS

Propanedinitrile, 2-(1,2,6-trimethyl-4(1H)-pyridinylidene)- (CA INDEX CN NAME)

- RN 49810-95-9 CAPLUS
- CN Propanedinitrile, 2-(1-buty1-2,6-dimethy1-4(1H)-pyridinylidene)- (CA INDEX NAME)

- RN 582297-74-3 CAPLUS
- CN Propanedinitrile, 2-[1-(2-ethylhexyl)-2,6-dimethyl-4(1H)-pyridinylidene]-(CA INDEX NAME)

- RN 582297-75-4 CAPLUS
- CN Propanedinitrile, 2-(1-dodecyl-2,6-dimethyl-4(1H)-pyridinylidene)- (CA INDEX NAME)

- RN 582297-76-5 CAPLUS
- $\label{eq:cn_sum} \mbox{CN} \quad \mbox{Propanedinitrile, } 2 [1 [3 [(2 \mbox{ethylhexyl}) \mbox{oxy}] \mbox{propyl}] 2, \\ 6 \mbox{dimethyl} 4 \mbox{(1H)} 2 \mbox{ethylhexyl}] 2 (1 [3 [(2 \mbox{ethylhexyl}) \mbox{oxy}] \mbox{propyl}] 2, \\ 6 \mbox{dimethyl} 4 \mbox{(1H)} 2 (1 [3 [(2 \mbox{ethylhexyl}) \mbox{oxy}] \mbox{propyl}] 2, \\ 6 \mbox{dimethyl} 4 \mbox{(1H)} 2 (1 [3 [(2 \mbox{ethylhexyl}) \mbox{oxy}] \mbox{propyl}] 2, \\ 6 \mbox{dimethyl} 4 \mbox{(1H)} 2 (1 [3 [(2 \mbox{ethylhexyl}) \mbox{oxy}] \mbox{propyl}] 2, \\ 6 \mbox{dimethyl} 2 (1 [3 [(2 \mbox{ethylhexyl}] \mbox{oxy}] \mbox{propyl}] 2, \\ 6 \mbox{dimethyl} 2 (1 [3 [(2 \mbox{ethylhexyl}] \mbox{oxy}] \mbox{ethylhexyl}] 2, \\ 6 \mbox{dimethyl} 2 (1 [3 [(2 \mbox{ethylhexyl}] \mbox{ethylhexyl}] \mbox{ethylhexyl}] 2, \\ 6 \mbox{ethylhexyl}] 2 (1 [3 [(2 \mbox{ethylhexyl}] \mbox{ethylhexyl}] \mbox{ethylhexyl}] 2, \\ 6 \mbox{ethylhexyl}] 2 (1 [3 [(2 \mbox{ethylhexyl}] \mbox{ethylhexyl}] \mbox{ethylhexyl}] 2, \\ 6 \mbox{ethylhexyl}] 2 (1 [3 [(2 \mbox{ethylhexyl}] \mbox{ethylhexyl}] \mbox{ethylhexyl}] 2, \\ 6 \mbox{ethylhexyl}] 2 (1 [3 [(2 \mbox{ethylhexyl}] \mbox{ethylhexyl}] \mbox{ethylhexyl}] 2, \\ 6 \mbox{ethylhexyl}] 2 (1 [3 [(2 \mbox{ethylhexyl}] \mbox{ethylhexyl}] \mbox{ethylhexyl}] 2, \\ 6 \mbox{ethylhexyl}] 2 (1 [3 [(2 \mbox{ethylhexyl}] \mbox{ethylhexyl}] \mbox{ethylhexyl}] 2, \\ 6 \mbox{ethylhexyl}] 2 (1 [3 [(2 \mbox{ethylhexyl}] \mbox{ethylhexyl}] 2, \\ 6 \mbox{ethylhexyl}] 2, \\ 6 \mbox{ethylhexyl}] 2 (1 [3 [(2 \mbox{ethylhexyl}] \mbox{ethylhexyl}] 2, \\ 6 \mbox{ethylhexyl}] 2, \\ 6 \mbox{ethylhexyl}] 2 (1 [3 [(2 \mbox{ethylhexyl}] \mbox{ethylhexyl}] 2, \\ 6 \mbox{ethylhexyl}] 2, \\ 6 \mbox{ethylhexyl}] 2 (1 [3 [(2 \mbox{ethylhexyl}] \mbox{ethylhexyl}] 2, \\ 6 \mbox{ethylhexyl}] 2, \\ 6 \mbox{et$

pyridinylidene]- (CA INDEX NAME)

- RN 582297-77-6 CAPLUS
- CN Propanedinitrile, 2-[2,6-dimethyl-1-(3,5,5-trimethylhexyl)-4(1H)-pyridinylidene]- (CA INDEX NAME)

- RN 582297-79-8 CAPLUS
- CN Propanedinitrile, 2,2'-[oxybis[2,1-ethanediyloxy-3,1-propanediyl(2,6-dimethyl-1(4H)-pyridinyl-4-ylidene)]]bis- (9CI) (CA INDEX NAME)

PAGE 1-B

- OS.CITING REF COUNT:
- THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD
- REFERENCE COUNT:

- (14 CITINGS)
- THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L5 ANSWER 9 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2003:608948 CAPLUS

DOCUMENT NUMBER: 139:395786

TITLE: Reaction of N1,N2-diarylamidines with

pyridinylidene]propanedinitriles

(2,3-diphenylcyclopropen-1-ylidene)propanedinitrile: Synthesis of [2-arylamino-4(1H)-

AUTHOR(S): Gomaa, Mohsen A.-M.; Doepp, Dietrich
CORPORATE SOURCE: Chemistry Department, Faculty of Science, Minia

CORPORATE SOURCE: Chemistry Department, Faculty of Science, University, El-Minia, 61519, Egypt

SOURCE: Synthesis (2003), (10), 1545-1548

CODEN: SYNTBF; ISSN: 0039-7881 PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:395786

AB A series of [1-aryl-2-arylamino-5,6-diphenyl-4(1H)pyridinylidene]propanedinitriles I (RI = H, Me; RZ = Me, OMe; RI = H; RZ =
t-Bu) has been synthesized by the reaction of NI,N2-diarylamidines with
(2,3-diphenylcyclopropen-1-ylidene)propanedinitrile. Structures of I have
been assigned on the basis of NNR spectra and NOE expts.

IT 625835-36-1P 625835-37-2P 625835-38-3P 625835-39-4P 625835-40-7P

Т

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of (arylaminopyridinylidene)propanedinitriles via ring-opening of (diphenylcyclopropenylidene)propanedinitrile followed by [3 + 3]-cycloaddn. with diarylamidines and dehydrogenation)

RN 625835-36-1 CAPLUS

CN Propanedinitrile, 2-[1-(4-methylphenyl)-6-[(4-methylphenyl)amino]-2,3-diphenyl-4(1H)-pyridinylidene]- (CA INDEX NAME)

- RN 625835-37-2 CAPLUS
- CN Propanedinitrile, 2-[1-(4-methoxyphenyl)-6-[(4-methoxyphenyl)amino]-2,3-diphenyl-4(1H)-pyridinylidene]- (CA INDEX NAME)

- RN 625835-38-3 CAPLUS
- CN Propanedinitrile, 2-[1-[4-(1,1-dimethylethyl)phenyl]-6-[[4-(1,1-dimethylethyl)phenyl]amino]-2,3-diphenyl-4(1H)-pyridinylidene]- (CA INDEX NAME)

- RN 625835-39-4 CAPLUS
- CN Propanedinitrile, 2-[3-methyl-1-(4-methylphenyl)-2-[(4-methylphenyl)amino]-5,6-diphenyl-4(1H)-pyridinylidene]- (CA INDEX NAME)

- RN 625835-40-7 CAPLUS
- CN Propanedinitrile, 2-[1-(4-methoxyphenyl)-2-[(4-methoxyphenyl)amino]-3-methyl-5,6-diphenyl-4(1H)-pyridinylidene]- (CA INDEX NAME)

OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD

(6 CITINGS)

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 10 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2001:664786 CAPLUS

DOCUMENT NUMBER: 136:20953

TITLE: Simple zwitterionic merocyanines as potential NLO

chromophores

AUTHOR(S): Kay, A. J.; Woolhouse, A. D.; Gainsford, G. J.; Haskell, T. G.; Wyss, C. P.; Giffin, S. M.; McKinnie,

I. T.; Barnes, T. H.

CORPORATE SOURCE: Industrial Research Limited, Lower Hutt, N. Z.

SOURCE: Journal of Materials Chemistry (2001),

11(9), 2271-2281

CODEN: JMACEP; ISSN: 0959-9428

PUBLISHER: Royal Society of Chemistry DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:20953

A suite of zwitterionic pyridylidene-based merocyanines that contain no interconnecting m-bridge between the donor and acceptor rings has been synthesized and their second-order NLO properties evaluated largely by semi-empirical computational methods (MOPAC 97/AM1). Contrary to expectation, increasing the degree of inter-ring twist (θ) , at least up to 55°, in these new pyridylideneazolone chromophores is found to have little or no effect on the figure of merit $[\mu\beta(0)]$. An X-ray crystallog. appraisal of one of these chromophores, , reveals however that the twist angle (albeit in the solid state) is greater than that predicted by computation and that all other features are consistent with the highly zwitterionic nature of these systems. In spite of this, a combination of factors-insufficient acceptor strength, insufficient extent of conjugation and perhaps insufficient twist angle, in particular clearly leads to the low values of the quadratic hyperpolarizabilities. The trade-off between targeting a more modest hyperpolarizability term from a min. of π -conjugating framework between donor and acceptor (and therefore synthetic expediency) and seeking a moderate-to-high dipole moment has therefore resulted in only low figures of merit for these systems. Calcns. performed on a suite of readily accessible, iscelectronic cyanines, in which the acceptor is a stabilized cyclopentadienide carbocycle rather than a heterocycle, have revealed the potential that these systems have as NLO chromophores. Representative polymer-tetherable derivs. of this system have been prepared as have the

corresponding TDI-based polyurethanes. IT 377743-32-3P

RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(light tan dye; preparation of simple zwitterionic merocyanines as potential NLO chromophores)

RN 377743-32-3 CAPLUS

CN

Propanedinitrile, 2-[1-(2,3-dihydroxypropyl)-4(1H)-pyridinylidene]- (CA INDEX NAME)

377743-37-8P

RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (yellow dye; preparation of simple zwitterionic merocyanines as potential NLO chromophores)

RN 377743-37-8 CAPLUS

CN Propanedinitrile, 2-[1-(2,3-dihydroxypropy1)-3,5-diiodo-4(1H)pyridinylidene] - (CA INDEX NAME)

OS.CITING REF COUNT:

THERE ARE 23 CAPLUS RECORDS THAT CITE THIS 23 RECORD (23 CITINGS)

REFERENCE COUNT:

40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 11 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

2001:57003 CAPLUS

ACCESSION NUMBER: DOCUMENT NUMBER: 134:107761

TITLE: Material for organic electroluminescent component

INVENTOR(S): Tamano, Michiko; Onikubo, Shunichi

PATENT ASSIGNEE(S): Toyo Ink Mfg. Co., Ltd., Japan SOURCE: Jpn. Kokai Tokkyo Koho, 22 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--------|------------|-----------------|------------|
| | | | | |
| JP 2001019946 | A | 20010123 | JP 1999-189859 | 19990705 < |
| PRIORITY APPLN. INFO.: | | | JP 1999-189859 | 19990705 < |
| OTHER SOURCE(S): | MARPAT | 134:107761 | | |
| | | | | |

AB The invention refers to a material for organic electroluminescent components I [R1,3 = single ring or condensed polycyclic; A = 0, or 1,2-substituted methylene where the substituents R3,4 = H, cyano, halo, alkyl-carbonyl, or alkoxycarbonyl, where both R3,4 may not be H].

IT 102654-01-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(material for organic electroluminescent component)

RN 102654-01-3 CAPLUS

CN Propanedinitrile, 2-(2,6-dimethyl-4(1H)-pyridinylidene)- (CA INDEX NAME)

CORPORATE SOURCE:

L5 ANSWER 12 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1999:451746 CAPLUS

DOCUMENT NUMBER: 131:287731

TITLE: Highly transparent and birefringent chromophores for

organic photorefractive materials
AUTHOR(S): Wortmann, R.; Glania, C.; Kramer, P.; Lukaszuk, K.;

Matschiner, R.; Twieg, R. J.; You, F.

Institute of Physical Chemistry, University of Mainz,

Mainz, D-55099, Germany SOURCE: Chemical Physics (1999), 245(1-3), 107-120

CODEN: CMPHC2: ISSN: 0301-0104

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal LANGUAGE: English

English A series of chromophores for application in organic photorefractive (PR) materials is investigated by electrooptical absorption measurements (EOAM). This exptl. technique yields information on the transition dipole moment µag, the ground-state dipole moment µg, and the change of the dipole moment upon optical excitation Au within the intense charge-transfer band of the dyes. It is shown that the results of the EOAM experiment allow us to estimate the PR figures-of-merit (FOMs) of the chromophores by either perturbational two-level equations or Kramers-Kroniq transformation. In particular, chromophores based on the heterocyclic dihydropyran and dihydropyridine groups in combination with dicyano and cyanocarboxy acceptor units were investigated. These donor-acceptor pairs yield chromophores close to the 'cyanine limit' that is characterized by a small dipole difference, but a large ground-state dipole moment and a large polarizability anisotropy. This leads to very high PR FOMs of the new PR chromophores that are demonstrated to be

superior to conventional second-order nonlinear optical chromophores in situations where the medium has a low glass transition.

T 49810-95-9 RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)

(transparent and birefringent chromophore for organic photorefractive materials)

RN 49810-95-9 CAPLUS

CN Propanedinitrile, 2-(1-butyl-2,6-dimethyl-4(1H)-pyridinylidene)- (CA INDEX NAME)

OS.CITING REF COUNT: 19 THERE ARE 19 CAPLUS RECORDS THAT CITE THIS

RECORD (19 CITINGS)

REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 13 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1998:490436 CAPLUS DOCUMENT NUMBER: 129:142690

ORIGINAL REFERENCE NO.: 129:29025a,29028a

ORIGINAL REFERENCE NO.: 129:29025a,29028a
TITLE: Liquid-crystal display device

INVENTOR(S): Dyer, Daniel John; Twieg, Robert James

PATENT ASSIGNEE(S): International Business Machines Corporation, USA

SOURCE: U.S., 8 pp.
CODEN: USXXAM

DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--------------------------|----------|-------------|------------------------|------------|
| | | | | |
| US 5783114 | A | 19980721 | US 1996-753841 | 19961202 < |
| PRIORITY APPLN. INFO.: | | | US 1996-753841 | 19961202 < |
| ASSIGNMENT HISTORY FOR U | JS PATEN | T AVAILABLE | IN LSUS DISPLAY FORMAT | |

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS OTHER SOURCE(S): MARPAT 129:142690

AB The present invention provides a liquid-crystal display device comprising a light-modulating composition comprising pyrimidine- or pyridazine-type liquid crystals preferably admixed with other liquid crystals disposed between two electrodes.

IT 204926-83-0 204926-84-1 204926-91-0 204926-97-6 204927-01-5 210641-60-4 210641-89-7 210641-96-6

RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses) $\,$

(liquid-crystal electrooptical display devices containing)

RN 204926-83-0 CAPLUS

CN Propanedinitrile, 2-[1-(4-hexylphenyl)-4(1H)-pyridinylidene]- (CA INDEX NAME)

RN 204926-84-1 CAPLUS

CN Propanedinitrile, 2-[1-[4-(1,1,2,2,3,3,4,4,5,5,6,6,6tridecafluorohexyl)phenyl]-4(1H)-pyridinylidene]- (CA INDEX NAME)

RN 204926-91-0 CAPLUS

CN Benzoic acid, 4-[4-(dicyanomethylene)-1(4H)-pyridinyl]-, decyl ester (CA INDEX NAME)

RN 204926-97-6 CAPLUS

CN Propanedinitrile, 2-[1-[4-[2-[4-(decyloxy)phenyl]ethynyl]phenyl]-4(1H)-pyridinylidene]- (CA INDEX NAME)

RN 204927-01-5 CAPLUS

CN Propanedinitrile, 2-[1-[4-[(1E)-2-[4-(decyloxy)phenyl]]diazenyl]phenyl]4(1H)-pyridinylidene]- (CA INDEX NAME)

Double bond geometry as shown.

RN 210641-60-4 CAPLUS

CN Benzoic acid, 4-[4-(dicyanomethylene)-1(4H)-pyridinyl]-, 1-methylheptyl ester (CA INDEX NAME)

RN 210641-89-7 CAPLUS

CN Propanedinitrile, 2-[1-[4-[(1E)-2-[4-(dodecyloxy)phenyl]diazenyl]phenyl]4(1H)-pyridinylidene]- (CA INDEX NAME)

Double bond geometry as shown.

$$\begin{array}{c} \text{NC} \\ \text{CN} \end{array}$$

RN 210641-96-6 CAPLUS

CN Propanedinitrile, 2-[1-[4-[(1E)-2-[4-[(1-methylheptyl)oxy]phenyl]diazenyl]phenyl]-4(1H)-pyridinylidene]- (CA INDEX NAME)

Double bond geometry as shown.

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD, ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 14 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1998:161539 CAPLUS DOCUMENT NUMBER: 128:250986

ORIGINAL REFERENCE NO.: 128:49569a

TITLE: A new class of liquid crystals:

methylene-1, 4-dihydropyridines
AUTHOR(S): Dver. Daniel J.: Lee. Victor Y.: Tw

AUTHOR(S): Dyer, Daniel J.; Lee, Victor Y.; Twieg, Robert J. CORPORATE SOURCE: IBM Almaden Research Center, San Jose, CA, 95120, USA

SOURCE: Liquid Crystals (1998), 24(2), 271-281

CODEN: LICRE6; ISSN: 0267-8292

PUBLISHER: Taylor & Francis Ltd.
DOCUMENT TYPE: Journal

LANGUAGE: English

AB A group of liquid crystal materials which contain the novel

methylene-1,4-dihydropyridine substructure were synthesized and their mesogenic properties examined Three main classes of liquid crystal compds. which differ in the structure of the aromatic core group (Ph, azobenzene and diphenylacetylene) attached to the N of the 1,4-dihydropyridine group were studied. The synthesis of the methylene-1,4-dihydropyridine group was accomplished in excellent yield by a Knoevenagel condensation of a 4-pyridone intermediate with an active methylene compound The liquid crystal materials prepared thus far which contain this methylene-1,4-dihydropyridine structure all possess broad enantiotropic smectic A phases and onne example also possesses a tilted smectic C phase. These mesogens may possess

useful properties such as high birefringence.

IT 204926-84-1P 204926-97-6P 204927-01-5P

204927-02-6P 204927-03-7P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(preparation and liquid crystal properties of)

RN 204926-84-1 CAPLUS

N Propanedinitrile, 2-[1-[4-(1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluorohexyl)phenyl]-4(1H)-pyridinylidene]- (CA INDEX NAME)

RN 204926-97-6 CAPLUS

CN Propanedinitrile, 2-[1-[4-[2-[4-(decyloxy)phenyl]ethynyl]phenyl]-4(1H)pyridinylidene|- (CA INDEX NAME)

RN 204927-01-5 CAPLUS

CN Propanedinitrile, 2-[1-[4-[(1E)-2-[4-(decyloxy)pheny1]]diazeny1]pheny1]4(1H)-pyridinylidene]- (CA INDEX NAME)

Double bond geometry as shown.

RN 204927-02-6 CAPLUS

CN Propanedinitrile, 2-[1-[4-[(1E)-2-[4-(octadecyloxy)phenyl]]diazenyl]phenyl]4(1H)-pyridinylidene]- (CA INDEX NAME)

Double bond geometry as shown.

RN 204927-03-7 CAPLUS

CN Propanedinitrile, 2-[1-[4-[(1E)-2-[4-[(2ethylhexyl)oxy]phenyl]diazenyl]phenyl]-4(1H)-pyridinylidene]- (CA INDEX NAME) Double bond geometry as shown.

- IT 204927-08-2P
 - RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 - (preparation and reactant in decyl (dicyanomethylene)pyridinylbenzoate preparation)
- RN 204927-08-2 CAPLUS
- CN Benzoic acid, 4-[4-(dicyanomethylene)-1(4H)-pyridinyl]- (CA INDEX NAME)

- IT 204926-83-0P 20492
 - 204926-83-0P 204926-90-9P 204926-91-0P 204926-92-1P 204927-00-4P
 - RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and thermal behavior of)
- RN 204926-83-0 CAPLUS
- CN Propanedinitrile, 2-[1-(4-hexylphenyl)-4(1H)-pyridinylidene]- (CA INDEX NAME)

- RN 204926-90-9 CAPLUS
- CN Benzoic acid, 4-[4-(dicyanomethylene)-1(4H)-pyridinyl]-, ethyl ester (CA INDEX NAME)

RN 204926-91-0 CAPLUS

CN Benzoic acid, 4-[4-(dicyanomethylene)-1(4H)-pyridinyl]-, decyl ester (CA INDEX NAME)

RN 204926-92-1 CAPLUS

CN Benzoic acid, 4-4-(dicyanomethylene)-1(4H)-pyridinyl]-, (1R)-1-methylheptyl ester (CA INDEX NAME)

Absolute stereochemistry.

RN 204927-00-4 CAPLUS

CN Propanedinitrile, 2-[1-[4-[2-[4-(hexyloxy)phenyl]diazenyl]phenyl]-4(1H)-pyridinylidene]- (CA INDEX NAME)

OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD (7 CITINGS)

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 15 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1997:314990 CAPLUS DOCUMENT NUMBER: 126:299643

ORIGINAL REFERENCE NO.: 126:57885a,57888a

Silver halide photographic element containing TITLE:

arvlhydrazine

INVENTOR(S): Delprato, Ivano; Cogliolo, Isabella

PATENT ASSIGNEE(S): Minnesota Mining and Manufacturing Co., USA

Eur. Pat. Appl., 13 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--------|------------|-----------------|------------|
| | | | | |
| EP 763771 | A1 | 19970319 | EP 1995-114618 | 19950918 < |
| R: DE, FR, GB, | IT | | | |
| PRIORITY APPLN. INFO.: | | | EP 1995-114618 | 19950918 < |
| OTUED COMPORTER. | MADDAT | 126.299643 | | |

OTHER SOURCE(S):

MARPAT 126:299643

ANRNR
1
G (CH $_2$) $_n$ - N $=$ CZ 1 Z 2

- ΔR The present invention relates to a silver halide photog, element comprising a support bearing at least one silver halide emulsion layer including neg. surface latent image-type silver halide grains in reactive association (prior to imagewise exposure) with a hydrazine compound represented by the formula I (A = arvl; G = CO, SO, SO2, PO2, PO3, or C=NR2; R, R1, R2 = H, alkyl of 1 to 6 carbon atoms, alkylsulfinyl of 1 to 6 carbon atoms, or trifluoroacetyl; n = an integer from 1 to 3; Z1, Z2 = an electron-withdrawing group). The silver halide photog, element can be developed with a conventional alkaline rapid access-type developer solution,
- at a pH value lower than 11.0, containing a developing agent and an auxiliary developing agent to give high-contrast images.
- 189037-69-2 RL: TEM (Technical or engineered material use); USES (Uses)
 - (high-contrast black-and-white silver halide photog, films for lithog, containing)
- RN 189037-69-2 CAPLUS
- CN 1(4H)-Pyridineacetic acid, 4-(dicyanomethylene)-, 2-[4-(1-methylethoxy)phenyl]hydrazide (CA INDEX NAME)

189037-68-1

RL: TEM (Technical or engineered material use); USES (Uses) (preparation and use in high-contrast black-and-white silver halide photog. films for lithog.)

RN 189037-68-1 CAPLUS

1(4H)-Pyridineacetic acid, 4-(dicyanomethylene)-, 2-(4-methoxyphenyl)hydrazide (CA INDEX NAME)

CN MeC -CN NH-NH-C-CH2

L5 ANSWER 16 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN ACCESSION NUMBER: 1991:101669 CAPLUS

DOCUMENT NUMBER: 114 - 101669

ORIGINAL REFERENCE NO.: 114:17325a,17328a

TITLE: Reaction of 4-methylthio- and 4-chloropyridinium salts with active methylene compounds

AUTHOR(S): Fujita, Reiko; Sakamura, Sachie; Tomisawa, Hiroshi

CORPORATE SOURCE: Tohoku Coll. Pharm., Sendai, 981, Japan

Annual Report of the Tohoku College of Pharmacy (SOURCE:

1989), (36), 117-22

CODEN: TYKNAQ; ISSN: 0495-7342 DOCUMENT TYPE: Journal

LANGUAGE: Japanese

Reaction of 4-methylthio- and 4-chloro-1-methylpyridinium iodides with

active methylene compds. such as Me malonate, Me cyanoacetate, and malononitrile in THF in the presence of sodium hydride gave

1,4-dihydro-1-methyl-4-alkylidenepyridines in 61.4-98.5% yields. Similar reaction of quinolinium salts gave the resp. 4-alkylidenequinolines. The 1H NMR spectrum of 4-dycyanomethylene-1,4-dihydro-1-methylpyridine is

compared with those of 1-methyl-4(1H)-pyridone and -thiopyridone.

16344-72-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 16344-72-2 CAPLUS

CN Propanedinitrile, 2-(1-methyl-4(1H)-pyridinylidene)- (CA INDEX NAME)

Me CN

> L5 ANSWER 17 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN 113:191288

ACCESSION NUMBER: 1990:591288 CAPLUS

DOCUMENT NUMBER:

ORIGINAL REFERENCE NO.: 113:32385a,32388a

TITLE: Cyclizations of cyanothioacetamide in the presence of

sulfur

AUTHOR(S): Gewald, K.; Schindler, R.

CORPORATE SOURCE: Sekt. Chem., Tech. Univ. Dresden, Dresden, DDR-8027, Ger. Dem. Rep.
SOURCE: Journal fuer P

Journal fuer Praktische Chemie (Leipzig) (1990

), 332(2), 223-8

CODEN: JPCEAO: ISSN: 0021-8383

DOCUMENT TYPE: Journal LANGUAGE: German

OTHER SOURCE(S):

CASREACT 113:191288

AB NCCHZCSNH2 (I) reacts with S in the presence of Bt3N to form the 2,5-diaminothiophene II and in the presence of Et0Na the 1,4-dihydropyridine derivative III. II easily undergoes ring opening to give Me 14300 CCC/NACCON LOCAL NEW 1500 CCC NACCON TO THE NAME OF THE PROPERTY OF THE NAME OF THE PROPERTY OF THE NAME OF

MeS(H2N)C:C(CN):C(SMe)NH2. Catalyzed by amine I, cyclic ketones, and S give the 2-spiro[thienc](2,3-d)pyrimidine-4-thiones] IV (n = 1,2). I reacts with S and RNCS (R = Me, Ph, ally1) to form

4-amino-4-thiazoline-2-thiones and with S and CS2 to yield

5-amino-1,2-dithiol-3-thione derivs. II and the aminothiazolinethiones can be converted into 5,6-heterocondensed pyrimidine-4-thiones.

130089-86-0P RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of) RN 130089-86-0 CAPLUS

OS.CITING REF COUNT: 14 THERE ARE 14 CAPLUS RECORDS THAT CITE THIS RECORD (14 CITINGS)

L5 ANSWER 18 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN ACCESSION NUMBER: 1989:173052 CAPLUS

DOCUMENT NUMBER: 110:173052

ORIGINAL REFERENCE NO.: 110:28701a,28704a

TITLE: Pyridinethiones. XV.

3-Methylthio-2-pentene-1,5-diones as synthons for 4-methylthio-2(1H)-pyridinethiones, and synthesis of

4-methylene-1, 4-dihydropyridines

AUTHOR(S): Becher, Jan; Hansen, Poul

Dep. Chem., Odense Univ., Odense, DK-5230, Den.

Journal of Heterocyclic Chemistry (1988),

25(4), 1129-34

CODEN: JHTCAD: ISSN: 0022-152X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 110:173052

SOURCE:

- RCOCH:C(SMe)CH2COR (I; R = 2-thienyl, 2-furyl, Ph, 4-MeC6H4, 4-MeOC6H4) AB were treated with Me3COK in Me2SO and then R1NCS (R1 = Ph, 4-ClC6H4, 4-MeOC6H4, 2-MeC6H4, 4-BrC6H4), followed by aqueous HC1 and heating in EtOH to give 16-78% the title pyridinethiones II (R, R1 = same). The S-alkylation of I with MeI or EtI and then condensation with NaCH(CN)2 gave methylenedihydropyridines III (R = Ph, 2-thienyl; R1 = Ph, 4-ClC6H4; R2 = Me, Et).
- 120105-26-2P 120105-47-7P 120105-48-8P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
- RN 120105-26-2 CAPLUS
- CN Propanedinitrile, 2-[1-(4-chlorophenyl)-2-(methylthio)-6-(2-thienyl)-3-(2thienvlcarbonvl)-4(1H)-pvridinvlidene]- (CA INDEX NAME)

- RN 120105-47-7 CAPLUS
- Propanedinitrile, 2-[3-benzoyl-2-(ethylthio)-1,6-diphenyl-4(1H)pyridinylidene]- (CA INDEX NAME)

RN 120105-48-8 CAPLUS

CN Propanedinitrile, 2-[3-benzoyl-2-(methylthio)-1,6-diphenyl-4(1H)pyridinylidene] - (CA INDEX NAME)

OS.CITING REF COUNT:

THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

ANSWER 19 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

2

ACCESSION NUMBER: 1988:602509 CAPLUS DOCUMENT NUMBER: 109:202509

ORIGINAL REFERENCE NO.: 109:33333a,33336a

TITLE: Crystal structures and electronic properties of

organic conductors based on AzaTCNQ AUTHOR(S): Urayama, Hatsumi; Inabe, Tamotsu; Mori, Takehiko;

Maruvama, Yusei; Saito, Gunzi

Inst. Mol. Sci., Okazaki, 444, Japan CORPORATE SOURCE:

SOURCE: Bulletin of the Chemical Society of Japan (

> 1988), 61(6), 1831-6 CODEN: BCSJA8; ISSN: 0009-2673

DOCUMENT TYPE: Journal

LANGUAGE:

English AB AzaTCNQ ((4-dicyanomethyl-1-pyridinio)dicyanomethanide) is employed as an organic acceptor to form new organic conductors with a TTF family such as TTF, TMTTF, TMTSF, HMTTF, and DBTTF. Among them, TMTTF and TMTSF give 2:1 single crystals and the latter affords the most conductive complex, showing a metallic characteristic down to 150 K. This can be observed by measuring the thermoelec. power and the ESR spectra. A crystal structure anal. indicates that only TMTSF mols. stack to form one-dimensional conduction pathways, while AzaTCNQ mols. are arranged side-by-side and oriented almost perpendicular to the donor mols. There exists an orientational disorder of the nitrogen atom in the pyridine skeleton of an AzaTCNQ mol., which may be associated with the weak temperature dependence of the

elec. conductivity 93179-09-0

RL: USES (Uses)

(in preparation of azaTCNQ-based organic conductors) 93179-09-0 CAPLUS
Pyridinium, 1-methyl-, salt with [4-(dicyanomethylene)-1(4H)-RN CN pyridinyl]propanedinitrile (1:1) (9CI) (CA INDEX NAME) CM 1 CRN 84662-81-7 CMF C11 H4 N5 CM CRN 694-56-4 CMF C6 H8 N 108793-76-6 108793-78-8 RL: PRP (Properties) (organic conductors, structure and elec. properties of) RN 108793-76-6 CAPLUS CN Propanedinitrile, [4-(dicyanomethylene)-1(4H)-pyridinyl]-, ion(1-), salt with 2-(4,5-dimethyl-1,3-diselenol-2-ylidene)-1,3-diselenole (1:2) (9CI) (CA INDEX NAME) CM 1 CRN 55259-49-9 CMF C10 H12 Se4 Se

Me

CRN 108793-75-5 CMF C11 H4 N5 . C10 H12 Se4

CM 3

CRN 84662-81-7 CMF C11 H4 N5

CM

CRN 73261-22-0 CMF C10 H12 Se4 CCI RIS

RN 108793-78-8 CAPLUS

CN Propanedinitrile, [4-(dicyanomethylene)-1(4H)-pyridinyl)-, ion(1-), salt with 2-(4,5-dimethyl-1,3-dithiol-2-ylidene)-4,5-dimethyl-1,3-dithiole (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 50708-37-7 CMF C10 H12 S4

Me S S Me

CM :

CRN 108793-77-7

```
CMF C11 H4 N5 . C10 H12 S4
```

3 CRN 84662-81-7 CMF C11 H4 N5

CN

CM 4

CRN 52597-32-7 CMF C10 H12 S4 CCI RIS



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

L5 ANSWER 20 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN 1987:617436 CAPLUS

107:217436

Journal

ACCESSION NUMBER: DOCUMENT NUMBER:

ORIGINAL REFERENCE NO.: 107:34875a,34878a TITLE:

AUTHOR(S):

CORPORATE SOURCE: SOURCE:

DOCUMENT TYPE: LANGUAGE:

OTHER SOURCE(S):

4-methylene-1, 4-dihydropyridines Asaad, Fahmy Mekhail; Becher, Jan; Moller, Jorgen; Varma, Karikath Sukumar Dep. Chem., Odense Univ., Odense, DK-5230, Den.

Pyridinethiones. XIV. Reactions of 2- and 4-alkylthiopyridines; synthesis of 1,6- and 2,7-naphthyridines via 2-methylene-1,2-dihydro- and

Synthesis (1987), (3), 301-4 CODEN: SYNTBF; ISSN: 0039-7881

English

CASREACT 107:217436

AB Pyridinium iodides I (R = Ph, p-ClC6H4, o-tolyl, p-anisyl; Rl = Me, SMe, SCH2Ph, OMe) reacted with active methylene compds. XCH2CN (X = CN, COZEt) to give 37-79% 8 methylenedhydropyridines II and III, which were cyclized by treatment with H3PO4 to give 73-81% 4 1,6- and 2,7-naphthyridines such as IV (R = Ph, p-anisyl).

ΙV

- RN 11123-13-8 CAPLUS
 CN Propanedinitrile, 2-[3-acetyl-6-methyl-2-(methylthio)-1-phenyl-4(1H)pyridinylidene]- (CA INDEX NAME)

- RN 111123-15-0 CAPLUS
- CN Propanedinitrile, 2-[3-acetyl-1-(4-methoxyphenyl)-6-methyl-2-(methylthio)-4(1H)-pyridinylidene]- (CA INDEX NAME)

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L5 ANSWER 21 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1987:416074 CAPLUS

DOCUMENT NUMBER: 107:16074

ORIGINAL REFERENCE NO.: 107:2579a,2582a
TITLE: New organic con-

TITLE: New organic conductors based on AzaTCNQ
AUTHOR(S): Urayama, H.: Saito, G.: Inabe, T.: Mori.

AUTHOR(S): Urayama, H.; Saito, G.; Inabe, T.; Mori, T.; Maruyama,

CORPORATE SOURCE: Inst. Solid State Phys., Univ. Tokyo, Tokyo, 106,

Japan SOURCE: Synthetic Metals (1987), 19(1-3), 469-74

CODEN: SYMEDZ: ISSN: 0379-6779

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Complexes of AzaTCNQ(4-dicyanomethylenepyridinium dicyanomethylide) with the TTF family were examined as a new candidate for organic conductors. The tetramethyltetraselenafulvalene complex had high conductivity, and the metallic character was confirmed by thermoelec.-power and ESR measurements. The stoichiometry is 2:1, and the structural study shows that only donor mols. form a 1-dimensional stack of conduction, while the AzaTCNQ mol. plane is oriented parallel to the donor stack. The orientational disorder of AzaTCNQ or resumbly causes the weak temperature dependence of charge transport.

IT 108793-70-0 108793-72-2 108793-74-4

108793-76-6 108793-78-8 RL: PRP (Properties)

(elec. conductive) RN 108793-70-0 CAPLUS

CN Propanedinitrile, [4-(dicyanomethylene)-1(4H)-pyridinyl]-, ion(1-), salt with 2-(1,3-dithiol-2-vlidene)-1,3-dithiole (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 35079-56-2 CMF C6 H4 S4 CCI RIS

RN 108793-72-2 CAPLUS CN Propanedinitrile, 14

Propanedinitrile, [4-(dicyanomethylene)-1(4H)-pyridiny1]-, ion(1-), salt with 2-(5,6-dihydro-4H-cyclopenta-1,3-dithiol-2-ylidene)-5,6-dihydro-4H-cyclopenta-1,3-dithiole (9CI) (CA INDEX NAME)

CM 1

CRN 57512-84-2 CMF C12 H12 S4

CM 2

CRN 108793-71-1 CMF C12 H12 S4 . C11 H4 N5

CM 3

CRN 57527-01-2 CMF C12 H12 S4 CCI RIS

RN 108793-74-4 CAPLUS

CN Propanedinitrile, [4-(dicyanomethylene)-1(4H)-pyridinyl)-, ion(1-), salt with 2-(1,3-benzodithiol-2-ylidene)-1,3-benzodithiole (9CI) (CA INDEX NAME)

CM 1

CRN 24648-13-3 CMF C14 H8 S4

CM 2

CRN 108793-73-3 CMF C14 H8 S4 . C11 H4 N5

CM 3

CRN 35079-60-8 CMF C14 H8 S4 CCI RIS

RN 108793-76-6 CAPLUS CN Propanedinitrile, [4

Propanedinitrile, [4-(dicyanomethylene)-1(4H)-pyridinyl]-, ion(1-), salt with 2-(4,5-dimethyl-1,3-diselenol-2-ylidene)-1,3-diselenole (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 55259-49-9 CMF C10 H12 Se4

CM 2

CRN 108793-75-5 CMF C11 H4 N5 . C10 H12 Se4

MF CII H4 N5 . CIU HIZ Se

CM 3

CRN 73261-22-0 CMF C10 H12 Se4 CCI RIS

RN 108793-78-8 CAPLUS

Propanedinitrile, [4-(dicyanomethylene)-1(4H)-pyridinyl]-, ion(1-), salt with 2-(4,5-dimethyl-1,3-dithiol-2-ylidene)-4,5-dimethyl-1,3-dithiole (1:2) (9CI) (CA INDEX NAME)

CM 1

CN

CRN 50708-37-7 CMF C10 H12 S4

CM

CRN 108793-77-7 CMF C11 H4 N5 . C10 H12 S4

> CM 3

CRN 84662-81-7

CMF C11 H4 N5

CRN 52597-32-7 CMF C10 H12 S4 CCI RIS

OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

ANSWER 22 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN ACCESSION NUMBER: 1985:462545 CAPLUS

DOCUMENT NUMBER: 103:62545

ORIGINAL REFERENCE NO.: 103:9945a,9948a

TITLE: Photoconductor compositions

PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan SOURCE: Jpn. Kokai Tokkyo Koho, 25 pp.

CODEN: JKXXAF DOCUMENT TYPE: Patent

> TETATO D3 mm

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: PATENT INFORMATION: DAMENIE NO

| FAIENI NO. | KIND | DAIL | AFFLICATION NO. | DAIL |
|--------------------------|----------|-------------|------------------------|------------|
| | | | | |
| JP 60083035 | A | 19850511 | JP 1983-191244 | 19831013 < |
| JP 02014696 | В | 19900409 | | |
| US 4598033 | A | 19860701 | US 1984-660572 | 19841012 < |
| PRIORITY APPLN. INFO.: | | | JP 1983-191244 A | 19831013 < |
| ASSIGNMENT HISTORY FOR U | IS PATEN | T AVAILABLE | IN LSUS DISPLAY FORMAT | |

ADDITORTON NO

D3 00 0

For diagram(s), see printed CA Issue. Photoconductor compns. contain a bisazo compound I [X = 0, S, Se, NR9; R = II, III, IV, V, CH(COMe)CONR13R14; R1-R4 = H, alkyl, aryl; R2R5 or R3R6 combination may complete a carbocyclic ring; R5,R6 = H when R2R5 or R3R6 rings are not formed; R7,R8 = electron attractive group; R7R8 may combine to form a ring; R9 = alkyl, aryl, aralkyl, alkenyl, alkynyl; R10 = CONR14R15, CO2R15; R11 = H, alkyl, Ph; R12 = H, lower alkyl, carbamoyl, CO2H, alkoxycarbonyl, aryloxycarbonyl; R13,R15 = H, alkyl, aryl, heterocycly1; R14 = H, alky1, Ph; A = aromatic or heterocyclic ring; m,n = 0,1,2]. Thus, VI, 4,4'-bis(diethylamino)-2,2'-dimethyltriphenylmethane and a polycarbonate resin were dissolved in CH2C12 and coated on a conductive film support to give an electrophotog, plate having good sensitivity.

97568-89-3

RL: USES (Uses)

(electrophotog, photoconductor compns, containing)

97568-89-3 CAPLUS

2-Naphthalenecarboxamide, 4,4'-[[1-butvl-4-(dicvanomethylene)-1,4-dihydro-2.6-pyridinediyl|bis(2.1-ethenediyl-4.1-phenyleneazo)|bis(N-(2fluorophenyl)-3-hydroxy- (9CI) (CA INDEX NAME)

OS.CITING REF COUNT: THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD 2 (2 CITINGS)

ANSWER 23 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1985:24036 CAPLUS DOCUMENT NUMBER: 102:24036 ORIGINAL REFERENCE NO.: 102:3951a,3954a

TITLE: Preparation and properties of AzaTCNO- anion salts and

mixed AzaTCNO-/TCNO -- salts of

N-alkylpyridinium and related cations AUTHOR(S): Tanaka, Hirohisa; Matsubayashi, Genetsu; Tanaka,

Toshio

CORPORATE SOURCE: Fac. Eng., Osaka Univ., Suita, 565, Japan SOURCE: Bulletin of the Chemical Society of Japan (

1984), 57(8), 2198-202

CODEN: BCSJA8: ISSN: 0009-2673

DOCUMENT TYPE: Journal

LANGUAGE: English [Cation] + ATCNQ--type salts [I; cation = N-alkylpyridinium,

AB

4-cyano-N-alkylpyridinium, (4-methyl-1-pyrazinio)dicyanomethanide, N-alkylquinolinium (alkyl = Me, Et), N-methylacridinium and -phenazinium; ATCNQ- = [4-(dicyanomethyl)-1-pyridinio]dicyanomethanide anion, so-called AzaTCNQ- anion] were prepared Elec. resistivities of these salts as

compacted samples were 106-109 Ωcm at 25°. [Cation]+

(ATCNQ-)0.1(TCNQ-)8.9 (cation = N-methyl- and N-ethylpyridinium, N-ethylquinolinium) and [N-methylquinolinium]+

(ATCNQ-)0.17(TCNQ--)0.83, whose elec. resistivities (104-106 Ωcm at 25°) are somewhat smaller than those of the corresponding

TCNQ-- salts, were also prepared Stackings of ATCNQ- and TCNQ--

```
anions are discussed on the basis of electronic reflectance and ESR
     spectra. I salts react with iodine in hexane to give I.Ix (cation =
     N-methyl- and N-ethylpyridinium and -quinolinium; x = 3.2-3.9), whose
     elec. resistivities (104-106 \Omegacm at 25°) are lower by a
     factor of 102-103 than those of the undoped I.
   93179-09-0P
                    93179-10-3P
                                    93179-11-4P
    93179-12-5P
                    93179-14-7P
                                    93179-15-8P
    93179-16-9P
                    93179-17-0P
                                    93179-18-1P
     93179-19-2P
                    93179-20-5P
                                    93179-21-6P
                    93179-23-8P
     93179-22-7P
                                    93179-24-9P
     93179-25-0P
                    93179-26-1P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation, spectra, and elec. conductivity of)
RN
    93179-09-0 CAPLUS
CN
    Pyridinium, 1-methyl-, salt with [4-(dicyanomethylene)-1(4H)-
    pyridinyl]propanedinitrile (1:1) (9CI) (CA INDEX NAME)
     CM
     CRN 84662-81-7
     CMF C11 H4 N5
    CM
    CRN 694-56-4
     CMF C6 H8 N
    93179-10-3 CAPLUS
RN
    Pyridinium, 1-ethyl-, salt with [4-(dicyanomethylene)-1(4H)-
CN
     pyridinyl]propanedinitrile (1:1) (9CI) (CA INDEX NAME)
    CM 1
     CRN 84662-81-7
     CMF C11 H4 N5
```

CRN 15302-96-2 CMF C7 H10 N

Εt

RN CN

93179-11-4 CAPLUS Pyridinium, 4-cyano-1-methyl-, salt with

[4-(dicyanomethylene)-1(4H)-pyridinyl]propanedinitrile (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 84662-81-7 CMF C11 H4 N5

C-CN CN

CM 2

CRN 13441-45-7 CMF C7 H7 N2

CN

93179-12-5 CAPLUS

Pyridinium, 4-cyano-1-ethyl-, salt with [4-(dicyanomethylene)-1(4H)-pyridinyl)propanedinitrile (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 84662-81-7 CMF C11 H4 N5

CM

CRN 45821-46-3 CMF C8 H9 N2

CN

93179-14-7 CAPLUS Pyrazinium, 1-(dicyanomethylene)-1,4-dihydro-4-methyl-, salt with [4-(dicyanomethylene)-1(4H)-pyridinyl]propanedinitrile (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 93179-13-6 CMF C8 H7 N4

```
CN
  C-CN
 Me
      CM
          2
      CRN 84662-81-7
      CMF C11 H4 N5
  C-CN
  CN
RN 93179-15-8 CAPLUS
CN Quinolinium, 1-methyl-, salt with [4-(dicyanomethylene)-1(4H)-
pyridinyl]propanedinitrile (1:1) (9CI) (CA INDEX NAME)
      CM
           1
      CRN 84662-81-7
```

CMF C11 H4 N5

CRN 21979-19-1 CMF C10 H10 N

RN 93179-16-9 CAPLUS

CN Quinolinium, 1-ethyl-, salt with [4-(dicyanomethylene)-1(4H)pyridinyl]propanedinitrile (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 84662-81-7 CMF C11 H4 N5

ĊN

CM

2 CRN 48122-97-0 CMF C11 H12 N

CN

93179-17-0 CAPLUS RN

Acridinium, 10-methyl-, salt with [4-(dicyanomethylene)-1(4H)-pyridinyl]propanedinitrile (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 84662-81-7 CMF C11 H4 N5

CM 2

CRN 13367-81-2 CMF C14 H12 N

RN 93179-18-1 CAPLUS

CN Phenazinium, 5-methyl-, salt with [4-(dicyanomethylene)-1(4H)pyridinyl)propanedinitrile (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 84662-81-7 CMF C11 H4 N5

CM 2

CRN 7432-06-6 CMF C13 H11 N2

RN 93179-19-2 CAPLUS

CN Pyridinium, 1-methyl-, salt with 2,2'-(2,5-cyclohexadiene-1,4-diylidene)bis[propanedinitrile], compd. with 1-methylpyridinium salt with [4-(dicyanomethylene)-1(4H)-pyridinyl]propanedinitrile (9CI) (CA INDEX NAME)

CM 1

CRN 93179-09-0

CMF C11 H4 N5 . C6 H8 N

CM 2

CRN 84662-81-7 CMF C11 H4 N5

CM

CRN 694-56-4 CMF C6 H8 N

Me N,

CM 4

CRN 34504-23-9 CMF C12 H4 N4 . C6 H8 N

CM 5

CRN 34507-61-4 CMF C12 H4 N4 CCI RIS

CM 6

CRN 694-56-4 CMF C6 H8 N

Me N+

RN 93179-20-5 CAPLUS CN Pyridinium, 1-ethy

Pyridinium, 1-ethyl-, salt with 2,2'-(2,5-cyclohexadiene-1,4-diylidene)bis[propanedinitrile] (1:1), compd. with 1-ethylpyridinium salt with [4-(dicyanomethylene)-1(4H)-pyridinyl]propanedinitrile (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 93179-10-3 CMF C11 H4 N5 . C7 H10 N

CM 2

CRN 84662-81-7 CMF C11 H4 N5

CN C CN CM 3 CRN 15302-96-2 CMF C7 H10 N

Et N+

CM 4

CRN 52700-09-1 CMF C12 H4 N4 . C7 H10 N

CM 5

CRN 34507-61-4 CMF C12 H4 N4 CCI RIS

NC- CN C- CN

CM

CRN 15302-96-2 CMF C7 H10 N

Et N+

CN

RN 93179-21-6 CAPLUS

Quinolinium, 1-methyl-, salt with 2,2'-(2,5-cyclohexadiene-1,4-diylidene)bis[propanedinitrile], compd. with 1-methylquinolinium salt with [4-(dicyanomethylene)-1(4H)-pyridinyl]propanedinitrile (9CI) (CA INDEX NAME)

CM 1

CRN 93179-15-8

CMF C11 H4 N5 . C10 H10 N

CRN 84662-81-7 CMF C11 H4 N5

CM 3

CRN 21979-19-1 CMF C10 H10 N

CM 4

CRN 34504-25-1 CMF C12 H4 N4 . C10 H10 N

CM 5

CRN 34507-61-4 CMF C12 H4 N4 CCI RIS

CRN 21979-19-1 CMF C10 H10 N

RN 93179-22-7 CAPLUS

CN Quinolinium, 1-ethyl-, salt with 2,2'-(2,5-cyclohexadiene-1,4-diylidene)bis[propanedinitrile], compd. with 1-ethylquinolinium salt with [4-(dicyanomethylene)-1(4H)-pyridinyl]propanedinitrile (9CI) (CA INDEX NAME)

CM 1

CRN 93179-16-9 CMF C11 H12 N . C11 H4 N5

CM

CRN 84662-81-7 CMF C11 H4 N5

CM 3

CRN 48122-97-0 CMF C11 H12 N

CM 4

```
CRN 50973-56-3
    CMF C12 H4 N4 . C11 H12 N
         CM
              5
         CRN 48122-97-0
         CMF C11 H12 N
         CM
             6
         CRN 34507-61-4
         CMF C12 H4 N4
CCI RIS
             CN
             C-CN
   CN
   93179-23-8 CAPLUS
   Pyridinium, 1-methyl-, salt with [4-(dicyanomethylene)-1(4H)-
    pyridinyl]propanedinitrile, compd. with iodine (9CI) (CA INDEX NAME)
    CM
        1
    CRN 7553-56-2
     CMF I2
I-I
    CM 2
    CRN 93179-09-0
     CMF C11 H4 N5 . C6 H8 N
         CM 3
         CRN 84662-81-7
         CMF C11 H4 N5
```

RN

CN

```
CM 4
             CRN 694-56-4
             CMF C6 H8 N
RN 93179-24-9 CAPLUS
CN Pyridinium, 1-ethyl-, salt with [4-(dicyanomethylene)-1(4H)-
pyridinyl]propanedinitrile, compd. with iodine (9CI) (CA INDEX NAME)
      CM
      CRN 7553-56-2
      CMF I2
I-I
      CM 2
      CRN 93179-10-3
      CMF C11 H4 N5 . C7 H10 N
             CM 3
             CRN 84662-81-7
CMF C11 H4 N5
```

```
CM 4
            CRN 15302-96-2
            CMF C7 H10 N
RN
    93179-25-0 CAPLUS
CN Quinolinium, 1-methyl-, salt with [4-(dicyanomethylene)-1(4H)-
pyridinyl]propanedinitrile, compd. with iodine (9CI) (CA INDEX NAME)
      CM
      CRN 7553-56-2
      CMF I2
I-I
      CM 2
      CRN 93179-15-8
      CMF C11 H4 N5 . C10 H10 N
            CM 3
            CRN 84662-81-7
CMF C11 H4 N5
```

```
CM 4
            CRN 21979-19-1
            CMF C10 H10 N
RN
    93179-26-1 CAPLUS
CN Quinolinium, 1-ethyl-, salt with [4-(dicyanomethylene)-1(4H)-
pyridinyl]propanedinitrile, compd. with iodine (9CI) (CA INDEX NAME)
      CM
      CRN 7553-56-2
      CMF I2
I-I
      CM 2
      CRN 93179-16-9
      CMF C11 H12 N . C11 H4 N5
            CM 3
```

CRN 84662-81-7 CMF C11 H4 N5

CM 4

CRN 48122-97-0 CMF C11 H12 N



IT 93179-28-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with pyridinium and quinolinium compds.)

RN 93179-28-3 CAPLUS

CN Propanedinitrile, [4-(dicyanomethylene)-1(4H)-pyridinyl]-, ion(1-), potassium (9CI) (CA INDEX NAME)

● K+

OS.CITING REF COUNT: 1

THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L5 ANSWER 24 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN ACCESSION NUMBER: 1983:118425 CAPLUS DOCUMENT NUMBER: 98:118425

```
ORIGINAL REFERENCE NO.: 98:17865a,17868a
TITLE:
                         Preparation and properties of AzaTCNQ- anion salts and
                         mixed AzaTCNQ-/TCNQ-/TCNQ salts of some
                         tetrakis(isocvanide)rhodium(I) cations, and x-ray
                         crystal structure of the
                         AzaTCNQ--tetrakis(2,6-dimethylphenyl
                         isocyanide)rhodium(I)+ salt
                         Matsubayashi, Genetsu; Tanaka, Hirohisa; Tanaka,
                         Toshio; Nakatsu, Kazumi
CORPORATE SOURCE:
                         Fac. Eng., Osaka Univ., Suita, 565, Japan
SOURCE:
                         Inorganica Chimica Acta (1982), 63(2),
                         217-24
                         CODEN: ICHAA3; ISSN: 0020-1693
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         English
    The following ATCNQ- salts and mixed ACTNQ-/TCNQ--/TCNQ salts (ATCNQ-
     = 4-dicyanomethylenepyridinium dicyanomethylide) of [Rh(RNC)4]+ were
     prepared: [Rh(RNC)4]+ATCNQ- (R = Ph, 2,6-Me2C6H3, and 2,4,6-Me3C6H2),
     [Rh(RNC)4]+(ATCNQ-)n(TCNQ-)1-n (R = 2,6-Me2C6H3, n = 0.2; R = Ph and
     2,4,6-Me3C6H2, n = 0.3), and [Rh(RNC)4]+(ATCNQ-)0.9(TCNQ-
     0.1(TCNO)0.8 (R = 2,6-Me2C6H3 and 2,4,6-Me3C6H2). Of these salts,
     [Rh(2,6-Me2C6H3NC)4]+(ATCNO-/TCNO-) and
     [Rh(2,6-Me2C6H3NC)4]+(ATCNO-/TCNO-/TCNO) exhibit elec. resistivities
     of .apprx.1 + 105 Ωcm as compacted samples at 25° and
     behave as typical semiconductors, while the resistivities of other salts
     are larger than 1 + 109 \Omegacm. Electronic absorption spectra
     and magnetic susceptibilities of the salts are discussed in terms of
     stackings of TCNQ.-, TCNQ, and ATCNQ- in the solid state. The crystal
     structure of [Rh(2,6-Me2C6H3NC)4]+ATCNQ- was determined by single-crystal x-ray
     diffraction. The triclinic crystal, space group P.hivin.1, has a
     10.964(2), b 12.768(2), c 8.375(1) Å, \alpha 102.03(2), \beta
     88.84(2), \gamma 112.07(2)°, and Z = 1, where the orientation of
     the ATCNO- is disordered with respect to the pyridinium ring.
     Least-squares refinement, based on 4094 independent reflections with [Fo]
     > 3\sigma(F), gave an R = 0.052.
    84662-83-9P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation, crystal structure, elec. resistance and magnetic
        susceptibility of)
RN
     84662-83-9 CAPLUS
    Rhodium(1+), tetrakis(2-isocyano-1,3-dimethylbenzene)-, (SP-4-1)-, salt
CN
     with [4-(dicyanomethylene)-1(4H)-pyridinyl]propagedinitrile (1:1) (9CI)
     (CA INDEX NAME)
     CM
         1
    CRN 84662-81-7
     CMF C11 H4 N5
```

CM :

CRN 61754-49-2 CMF C36 H36 N4 Rh CCI CCS

IT 84662-82-8DP, solid solution with tetrakis (phenylisocyanide) rhodium TONQ 84662-82-8P 84662-83-9DP, solid solution with tetrakis (dimethylphenylisocyanide) rhodium TCNQ 84662-84-0P RL: SPN (Synthetic preparation), PREP (Preparation) (preparation, elec. resistance and magnetic susceptibility of) RN 84662-82-8 (CapUISC.

RN 84662-82-8 CAPLUS
CN Rhodium(1+), tetrakis(isocyanobenzene)-, (SP-4-1)-, salt with [4-(dicyanomethylene)-1(4H)-pyridinyl]propanedinitrile (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 84662-81-7 CMF C11 H4 N5

CM 2

CRN 56192-48-4 CMF C28 H20 N4 Rh CCI CCS

$$Ph - N \stackrel{+}{=} C \stackrel{-}{=} N \stackrel{+}{+} Ph$$

$$Ph - N \stackrel{+}{=} C \stackrel{-}{=} Rh \stackrel{+}{+} \stackrel{-}{C} \stackrel{-}{=} N \stackrel{+}{+} Ph$$

$$C \stackrel{-}{=} N \stackrel{+}{+} Ph$$

RN 84662-82-8 CAPLUS CN Rhodium(1+), tetral

Rhodium(1+), tetrakis(isocyanobenzene)-, (SP-4-1)-, salt with [4-(dicyanomethylene)-1(4H)-pyridinyl]propanedinitrile (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 84662-81-7 CMF C11 H4 N5

CM 2

CRN 56192-48-4 CMF C28 H20 N4 Rh

CCI CCS

$$Ph-N \xrightarrow{+} C \xrightarrow{-} Rh \xrightarrow{+} C \xrightarrow{-} N \xrightarrow{+} Ph$$

$$C \xrightarrow{-} N \xrightarrow{+} Ph$$

$$C \xrightarrow{-} N \xrightarrow{+} Ph$$

RN 84662-83-9 CAPLUS

CN Rhodium(1+), tetrakis(2-isocyano-1,3-dimethylbenzene)-, (SP-4-1)-, salt with [4-(dicyanomethylene)-1(4H)-pyridinyl)propanedinitrile (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 84662-81-7 CMF C11 H4 N5

CM 2

CRN 61754-49-2 CMF C36 H36 N4 Rh CCI CCS

RN 84662-84-0 CAPLUS

 $\begin{array}{ll} \hbox{CN} & \hbox{Rhodium(1+), tetrakis(2-isocyano-1,3,5-trimethylbenzene)-, (SP-4-1)-, salt with $[4-(dicyanomethylene)-1(4H)-pyridinyl]propanedinitrile (1:1) (9CI) } \end{array}$

(CA INDEX NAME)

CM 1

CRN 84662-81-7 CMF C11 H4 N5

CM 2

CRN 70443-06-0 CMF C40 H44 N4 Rh CCI CCS

$$\begin{array}{c} \text{Me} \\ \text{Me} \\ \text{Me} \\ \text{N} \end{array} \begin{array}{c} - \\ \text{N} \end{array} \begin{array}{c} \text{N} \\ \text{N} \end{array} \begin{array}{c} - \\ \text{N} \end{array} \begin{array}{c} + \\ \text{N} \end{array} \begin{array}{c} - \\ \text{N} \end{array} \begin{array}{c} + \\ \text{Me} \\ \text{Me} \end{array} \begin{array}{c} - \\ \text{Me} \end{array} \begin{array}{c} - \\ \text{Me} \end{array} \begin{array}{c} - \\ \text{Me} \\ \text{Me} \end{array} \begin{array}{c} - \\ \text{Me} \end{array} \begin{array}{c}$$

IT 84662-84-0DP, solid solution with

tetrakis(trimethylphenylisocyanide)rhodium TCNQ

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, elec. resistance and magnetic susceptibility of,)

RN 84662-84-0 CAPLUS

Rhodium(1+), tetrakis(2-isocyano-1,3,5-trimethylbenzene)-, (SP-4-1)-, salt with (4-(dicyanomethylene)-1(4H)-pyridinyl)propanedinitrile (1:1) (9CI) (CA INDEX NAME)

CM 1

CN

CRN 84662-81-7

CM 2

CRN 70443-06-0 CMF C40 H44 N4 Rh CCI CCS

OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

L5 ANSWER 25 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN ACCESSION NUMBER: 1981:433460 CAPLUS

DOCUMENT NUMBER:

95:33460

SOURCE:

ORIGINAL REFERENCE NO.: 95:5629a,5632a

TITLE: Electrically photosensitive particles for electrophoretic migration imaging processes,

dispersions of these particles and processes using such dispersions Merrill, Stewart Henry; Turnblom, Ernest Wayne;

INVENTOR(S):

Stahly, Frederick August; Wright, Beth George; Wright, Hal Eldon

PATENT ASSIGNEE(S):

Eastman Kodak Co., USA Eur. Pat. Appl., 68 pp. CODEN: EPXXDW

DOCUMENT TYPE: Patient. LANGUAGE: English FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

| | PA? | TENT : | NO. | | | KIND | DATE | AP | PLICATION NO | | DATE | |
|-----|------|--------|------|------|------|---------|-------------|-----|--------------|--------|----------|---|
| | | | | | | | | | | | | |
| | EP | 2416 | 9 | | | A2 | 19810225 | EP | 1980-302706 | | 19800807 | < |
| | EP | 2416 | 9 | | | A3 | 19811125 | | | | | |
| | | R: | CH, | DE, | FR, | GB | | | | | | |
| | US | 4322 | 487 | | | A | 19820330 | US | 1979-64972 | | 19790808 | < |
| | CA | 1143 | 204 | | | A1 | 19830322 | CA | 1980-357297 | | 19800730 | < |
| | JP | 5603 | 0159 | | | A | 19810326 | JP | 1980-108369 | | 19800808 | < |
| RIO | RIT | Y APP | LN. | INFO | . : | | | US | 1979-64972 | A | 19790808 | < |
| SSI | GNME | ENT H | ISTO | RY F | OR U | S PATEN | T AVAILABLE | IN: | LSUS DISPLAY | FORMAT | | |

PR: AS GT

Ι

- AB Elec. photosensitive dispersion for electrophoretic imaging consists of a colorant and a polymeric binder comprising units containing ≥1 structures of triarylamine, p-aminotetraarylmethane,
 - 4, 4'-bis(p-amino)triarylmethane, 1, 1-bis(p-aminoaryl)isobutane,
 - 1,1-bis(p-aminoaryl)cyclohexane, N-alkyl-N,N-diarylamine,
 - N-alkenyl-N, N-diarylamine, N, N-diallyl-N-arylamine, and C3-12 heterocyclic containing ≥1 N atom in the ring structure. Thus,
 - polv(di-p-tolvlaminostyrene) 0.255 was mixed with a solution containing I
- 0.045. CH2Cl2 20 g, combined with Isopar G 225 mL, centrifuged, to give a precipitate (containing 15% of I), 0.26 g of which was milled 3 h with vinyltoluene-lauryl methacrylate-Li methacrylate-methacrylic acid polymer 0.26, Isopar G 4.65, and imaged in an imaging apparatus (Carousel projector with W lamp, imaging electrode 12.5-50 cm, voltage -1.5 kV) to give an image with Dmax and Dmin
- 1.42 and 0.08, resp., vs. 0.54 and 0.15 for a binder-free control. 65833-38-7
- RL: USES (Uses)
- (photoelectrophoretic imaging dispersion containing polymeric binder and) RN 65833-38-7 CAPLUS
- Propanedinitrile, 2-[2,6-bis[2-[4-(diethylamino)-2-methoxyphenyl]ethenyl]-CN 1-(phenylmethyl)-4(1H)-pyridinylidene)- (CA INDEX NAME)

OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)

L5 ANSWER 26 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1979:430527 CAPLUS

DOCUMENT NUMBER: 91:30527

ORIGINAL REFERENCE NO.: 91:4883a,4886a

TITLE: Photoelectrophoretic particles for producing color images

INVENTOR(S): Vanallan, James Albert; Webster, Frank Glenn;

Reynolds, George Arthur PATENT ASSIGNEE(S): Eastman Kodak Co., USA SOURCE: Ger. Offen., 74 pp. CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | | DATE |
|------------------------|------|----------|-----------------|---|------------|
| DE 2831054 | A1 | 19790118 | DE 1978-2831054 | _ | 19780714 < |
| DE 2831054 | B2 | 19820107 | | | |
| DE 2831054 | C3 | 19820812 | | | |
| US 4145215 | A | 19790320 | US 1977-816128 | | 19770715 < |
| US 4146707 | A | 19790327 | US 1978-874078 | | 19780201 < |
| CA 1110898 | A1 | 19811020 | CA 1978-305192 | | 19780612 < |
| FR 2397659 | A1 | 19790209 | FR 1978-20765 | | 19780712 < |
| FR 2397659 | B1 | 19800404 | | | |
| JP 54021722 | A | 19790219 | JP 1978-85243 | | 19780714 < |
| GB 2002528 | A | 19790221 | GB 1978-30093 | | 19780717 < |
| GB 2002528 | В | 19820127 | | | |
| PRIORITY APPLN. INFO.: | | | US 1977-816128 | A | 19770715 < |
| GT | | | | | |

- Elec. photosensitive particles for a photoelectrophoretic imaging device AB have the structure I (X is O, S, Se, or NR, where R = halogen, OH, alkoxy, or aryloxy substituted alkyl, aryl, aralkyl, cycloalkyl, alkenyl, or alkynyl; R5, R6 = CN or taken together form an O-substituted cyclic ring, other heterocyclic ring, or electron acceptor group; R1, R2 = alkyl, aryl, CL1(=CL2CL3=)mA1, CL4=CL5(CL3=CL7)n A2, or R1 is the same as R4 or R2 is the same as R3 in the completion of an alkylene bridge, where m and n = 0, 1, or 2; L1, L2, L3, L4, L5, L6, and L7 = H, alkyl, or aryl, or L3 or L4 is the same as R3 or R4 for completion of a carbocyclic ring; A1 and A2 are basic heterocyclic groups; R3 is H or the same as R2, L1, or L4 in a 5- or 6-membered carbocyclic ring; R4 is H or the same as R1, L1, or L4 in a 5- or 6-membered carbocyclic ring). Thus, an excellent red-brown image was produced by a known electrophoretic imaging method with the use of a dispersion containing II.
 - 65833-38-7 65833-47-8 65833-48-9 70503-51-4

RL: USES (Uses)

(electrophoretic color imaging composition containing elec. photosensitive particles of)

RN 65833-38-7 CAPLUS

CN Propanedinitrile, 2-[2,6-bis[2-[4-(diethylamino)-2-methoxyphenyl]ethenyl]-1-(phenylmethyl)-4(1H)-pyridinylidenel- (CA INDEX NAME)

$$\begin{array}{c} \operatorname{Et}_2 \operatorname{N} & \operatorname{CH}_2 - \operatorname{Ph} & \operatorname{NEt}_2 \\ \\ \operatorname{OMe} & \operatorname{CH} - \operatorname{CH} - \operatorname{CH} - \operatorname{CH} \\ \\ \operatorname{C} - \operatorname{CN} & \operatorname{CN} \end{array}$$

RN 65833-47-8 CAPLUS CN

Propanedinitrile, 2-[2,6-bis[2-[4-(dimethylamino)phenyl]ethenyl]-1-(phenylmethyl)-4(1H)-pyridinylidenel- (CA INDEX NAME)

RN 65833-48-9 CAPLUS

CN Propanedinitrile, 2-[1-butyl-2,6-bis[2-[4-(dimethylamino)phenyl]ethenyl]-4(1H)-pyridinylidene]- (CA INDEX NAME)

RN 70503-51-4 CAPLUS

CN Propanedinitrile, 2-[1-(phenylmethyl)-2,6-bis[2-(2,3,6,7-tetrahydro-1H,5Hbenzo[ij]quinolizin-9-yl)ethenyl]-4(1H)-pyridinylidene]- (CA INDEX NAME)

THERE ARE 9 CAPLUS RECORDS THAT CITE THIS RECORD

(9 CITINGS)

ANSWER 27 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN ACCESSION NUMBER: 1978:128987 CAPLUS

9

DOCUMENT NUMBER: 88:128987 ORIGINAL REFERENCE NO.:

88:20171a,20174a

TITLE: Migration imaging process

AUTHOR(S): Van Allan, James Albert; Webster, Frank Glenn;

Revnolds, George Arthur CORPORATE SOURCE: UK

SOURCE: Research Disclosure (1977), 162, 26-31 (No.

16247)

CODEN: RSDSBB; ISSN: 0374-4353

DOCUMENT TYPE: Journal; Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

OS.CITING REF COUNT:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|------------|
| | | | | |
| RD 162047 | | 19771010 | RD 1977-162047 | 19771010 < |
| PRIORITY APPLN. INFO.: | | | RD 1977-162047 | 19771010 < |
| GI | | | | |

AB Forty electrophotosensitive pigments of the structure I (R, R1 are heterocyclic nuclei linked through a system of conjugated double bonds, R2, R3 are H or together with R and R1, resp., form a carbocyclic ring; R4, R5 are electron-withdrawing groups or together form an acidic heterocycle as in merocyanine dyes; and X is 0, S, or NR6 where R6 is alkyl, aryl, aralkyl, or the like) are described for use in electrophoretic migration imaging. Thus, to 5g of an imaging dispersion containing Isopar G 2.2, Solvesso 1.3, Piccotex 100 1.4, and lauryl methacrylate-Li methacrylate-methacrylic acid-vinyltoluene polymer 0.1q was added II 0.45 q and the dispersion then milled with stainless steel balls for 3 h. Upon testing this dispersion in a migration imaging process, a neg. of an original was obtained on 1 electrode and a complementary image on the other electrode.

65833-38-7 65833-47-8 65833-48-9 RL: USES (Uses)

(electrophotosensitive pigment, for migration imaging process) 65833-38-7 CAPLUS

RN

CN Propanedinitrile, 2-[2,6-bis[2-[4-(diethylamino)-2-methoxyphenyl]ethenyl]-1-(phenylmethyl)-4(1H)-pyridinylidene]- (CA INDEX NAME)

$$\begin{array}{c} \text{CH}_2\text{-Ph} \\ \text{OMe} \\ \text{OMe} \\ \text{C} \\ \text{C} \\ \text{CN} \\ \end{array}$$

RN 65833-47-8 CAPLUS

CN Propanedinitrile, 2-[2,6-bis[2-[4-(dimethylamino)phenyl]ethenyl]-1-(phenylmethyl)-4(1H)-pyridinylidene|- (CA INDEX NAME)

RN

ANSWER 28 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN 1977:601414 CAPLUS

ACCESSION NUMBER: DOCUMENT NUMBER:

87:201414

ORIGINAL REFERENCE NO.:

87:31890h,31891a

TITLE:

N-Oxides and related compounds. Part 56. Preparation of NN'-linked bi(heteroarvls) from dehydroacetic acid and 2,6-dimethyl-4-pyrone

AUTHOR(S): Afridi, A. Sultan; Katritzky, Alan R.; Ramsden,

Christopher A.

CORPORATE SOURCE:

Sch. Chem. Sci., Univ. East Anglia, Norwich, UK Journal of the Chemical Society, Perkin Transactions

SOURCE:

1: Organic and Bio-Organic Chemistry (1972-1999) (1977), (12), 1428-36

CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: LANGUAGE:

Journal English

OTHER SOURCE(S): CASREACT 87:201414 GI

AB Cyclocondensation reactions of dehydroacetic acid (I) or 2,6-dimethyl-4-pyrone (II) with aminopyridones, aminotriazoles, and hydrazines gave N, N'-linked bi(heteroaryls). E.g., 4-amino-1, 2, 4-triazole with I and II gave 65% and 40% triazolylpyridone III, resp. 1-Amino-2-pyridone with II gave 15% bipyridinedione IV. NH2NH2.H2O with I gave 90% azine V. Reactions of III and related mono- and dications were studied.

II 62071-85-6P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and acetylation of)

- RN 62071-85-6 CAPLUS
- CN Propanedinitrile, 2-(1-amino-2,6-dimethyl-4(1H)-pyridinylidene)- (CA INDEX NAME)

- RN 64804-43-9 CAPLUS
- CN Benzamide, N-[4-(dicyanomethylene)-2,6-dimethyl-1(4H)-pyridinyl]- (CA INDEX NAME)

- RN 64804-44-0 CAPLUS

RN 64804-45-1 CAPLUS

Propanedinitrile, 2-[2,6-dimethyl-1-(4H-1,2,4-triazol-4-yl)-4(1H)-pyridinylidene]- (CA INDEX NAME)

CN

OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)

L5 ANSWER 29 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1977:105314 CAPLUS DOCUMENT NUMBER: 86:105314

ORIGINAL REFERENCE NO.: 86:16609a,16612a

TITLE: Charge-transfer π complexes formed from the

pyrylium ion
AUTHOR(S): Van Allan, James A.; Chang, Jack C.; Costa, Lorenzo

F.; Reynolds, George A.

CORPORATE SOURCE: Res. Lab., Eastman Kodak Co., Rochester, NY, USA

SOURCE: Journal of Chemical and Engineering Data (1977

), 22(1), 101-4 CODEN: JCEAAX; ISSN: 0021-9568

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

AB New organic charge-transfer compds. were prepared from an organic cation (I; R

H, X = S, X2 = ClO4; R = H, Me, X = O, X1 = BF4, ClO4, iodo) and a neutral organic mol. (triphenylamine or N-amino-4-(dicyanomethylene)-2,6-dimethyl-1,4-dihydropyridine). The absorption spectra of these charge-transfer complexes were determined in solution and in the solid state. These salts have the charge-transfer band in the visible region as a result of electron transfer from the organic molety to the cation. The extinction coefficient, association constant, conductivity, photocond., and emission were examined for a few

members of this series.

IT 62071-86-7P 62071-89-0P 62071-90-3P

62071-93-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and luminescence property of)

RN 62071-86-7 CAPLUS

CN Thiopyranium, 2,4,6-triphenyl-, perchlorate, compd. with 2-(1-amino-2,6-dimethyl-4(1H)-pyridinylidene)propanedinitrile (1:1:1) (CA INDEX NAME)

CM 1

CRN 62071-85-6 CMF C10 H10 N4

CM 2

CRN 2930-37-2 CMF C23 H17 S . C1 O4

CM 3

CRN 18342-83-1 CMF C23 H17 S

CM

CRN 14797-73-0 CMF C1 04

RN 62071-89-0 CAPLUS

 $\begin{array}{lll} \text{CN} & & \text{Pyrylium, } 4-(4-\text{methylphenyl})-2, 6-\text{diphenyl-, perchlorate, compd. with} \\ & 2-(1-\text{amino-2}, 6-\text{dimethyl-4(1H)-pyridinylidene)propanedinitrile (1:1:1)} \end{array}$

INDEX NAME)

CM 1

CRN 62071-85-6 CMF C10 H10 N4

NH₂

CN

CM 2

CRN 3558-64-3 CMF C24 H19 O . C1 O4

CM

CRN 47454-43-3 CMF C24 H19 O

Me Me

CM

CRN 14797-73-0 CMF C1 O4

0... 0... 0..

o== c1-o-

RN 62071-90-3 CAPLUS
CN Pyrylium, 4-(3-methylphenyl)-2,6-diphenyl-, tetrafluoroborate(1-), compd.
with (1-amino-2,6-dimethyl-4(1H)-pyridinylidene)propanedinitrile (1:1)

(9CI) (CA INDEX NAME)

CM 1

CRN 62071-85-6

CMF C10 H10 N4

NH2

CN

CM 2

CRN 61669-49-6 CMF C24 H19 O . B F4

CM

CRN 61669-48-5 CMF C24 H19 O

CM

CRN 14874-70-5 CMF B F4

CCI CCS

RN 62071-93-6 CAPLUS

Pyrylium, 4-(2-methylphenyl)-2,6-diphenyl-, perchlorate, compd. with 2-(1-amino-2,6-dimethyl-4(1H)-pyridinylidene)propanedinitrile (1:1:1) (CA INDEX NAME)

CM 1 CRN 62071-85-6 CMF C10 H10 N4 NH2 CN CM 2 CRN 62071-92-5 CMF C24 H19 O . C1 O4 CM 3 CRN 62071-91-4 CMF C24 H19 O CM CRN 14797-73-0 CMF C1 04

IT 62071-87-8P 62071-88-9P 62287-21-2P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 62071-87-8 CAPLUS

CN Pyrylium, 2,4,6-triphenyl-, tetrafluoroborate(1-), compd. with (1-amino-2,6-dimethyl-4(1H)-pyridinylidene) propanedinitrile (1:1) (9CI)

```
(CA INDEX NAME)
    CM 1
    CRN 62071-85-6
    CMF C10 H10 N4
     NH2
          Me
      C-CN
     CN
    CM
         2
    CRN 448-61-3
    CMF C23 H17 O . B F4
         CM
              3
         CRN 15959-35-0
         CMF C23 H17 O
          Ph
     0,+
     Ph
         CM
         CRN 14874-70-5
         CMF B F4
         CCI CCS
    3+
-F- B-
```

Me.

Ph.

INDEX NAME) CM 1

CN

62071-88-9 CAPLUS

Pyrylium, 2,4,6-triphenyl-, perchlorate, compd. with

2-(1-amino-2,6-dimethyl-4(1H)-pyridinylidene)propanedinitrile (1:1:1) (CA

```
CRN 62071-85-6
     CMF C10 H10 N4
      NH2
Me
            Me
      N.
      CN
     CM
           2
     CRN 1484-88-4
     CMF C23 H17 O . C1 O4
           CM
                3
           CRN 15959-35-0
           CMF C23 H17 O
Ph.
      0.+
            Ph
      Ph
           CM
           CRN 14797-73-0
           CMF C1 04
     62287 - 21 - 2 CAPLUS Pyrylium, 2,4,6-triphenyl-, iodide, compd. with
RN
CN
```

INDEX NAME)

CM 1

CRN 62287-20-1

CMF C20 H14 N4

2-(1-amino-2,6-diphenyl-4(1H)-pyridinylidene)propanedinitrile (1:1:1) (CA

CMF C23 H17 O . I

• I-

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L5 ANSWER 30 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER:
                       1975:170771 CAPLUS
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DOCUMENT NUMBER: 82:170771 ORIGINAL REFERENCE NO.: 82:27289a,27292a

TITLE: Heterocycles by cycloaddition. I.

Cycloaddition-extrusion-ring expansion reactions of five-membered mesoionic compounds with

diphenylcyclopropenone and related compounds.

Preparation of six-membered heterocycles

Matsukubo, Hiroshi; Kato, Hiroshi

Dep. Chem., Shinshu Univ., Matsumoto, Japan

Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (

1975), (7), 632-5 CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal English

LANGUAGE:

CORPORATE SOURCE:

AUTHOR(S):

SOURCE:

GI For diagram(s), see printed CA Issue.

MeNBzCHPhCO2H with Ac2O cyclized to the mesoionic oxazolone I which with the cyclopropenylidene derivs. II [R = 0, S, NSO2C6H4Me-p, C(CN)2, C(CN)CO2Et] gave 41-65% of the corresponding pyridine derivs. III. The thiazolone IV with II also gave III. The mesolonic dithiolone V with II [R = C(CN)CO2Et] gave the expected thiopyran derivative VI and the indenothiopyran VII.

54133-10-7P 56197-87-6P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 54133-10-7 CAPLUS CN Propanedinitrile, 2-(1-methyl-2,3,5,6-tetraphenyl-4(1H)-pyridinylidene)-(CA INDEX NAME)

- 56197-87-6 CAPLUS RN
- CN Propanedinitrile, 2-[1-methyl-2-(4-nitrophenyl)-3,5,6-triphenyl-4(1H)pyridinylidene] - (CA INDEX NAME)

OS.CITING REF COUNT: THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD 2 (2 CITINGS)

ANSWER 31 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1975:156017 CAPLUS DOCUMENT NUMBER: 82:156017

ORIGINAL REFERENCE NO.: 82:24889a,24892a

TITLE: Reactions of triafulvenes with azomethine vlides

AUTHOR(S): Eicher, Th.; Schaefer, V.

CORPORATE SOURCE: Inst. Org. Chem., Univ. Wuerzburg, Wuerzburg, Fed.

Rep. Ger.

SOURCE: Tetrahedron (1974), 30(22), 4025-9 CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

LANGUAGE: German GI

For diagram(s), see printed CA Issue.

AB The reaction of the azomethine ylides I (R = Me, Ph, R1 = Me, R2= Ph; R = R2 = Me, R1 = Ph), prepared by heating RCONR1CHR2CO2H with Ac2O, with cyclopropenones II (R3 = R4 = Ph, X = O, S; R3 = Me, Ph, R4 = Me, X = O) and of I (R = R2 =Ph, R1 = Me) with methylenecyclopropenes III (R5 = R6 = CN, COMe, COPh; R5 = CN, R6 = COPh, CO2Me) gave 4-pyridones IV and 1,4-dihydro-N-methyl-4-methylenepyridines V, resp., by (3 + 3) cycloaddn. The merocyanine systems V exhibited solvatochromic and thermochromic properties.

54133-10-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

- RN 54133-10-7 CAPLUS
- CN Propanedinitrile, 2-(1-methyl-2,3,5,6-tetraphenyl-4(1H)-pyridinylidene)-

OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

L5 ANSWER 32 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN ACCESSION NUMBER: 1974:504800 CAPLUS

DOCUMENT NUMBER: 81:104800

ORIGINAL REFERENCE NO.: 81:16563a,16566a

TITLE: Cycloaddition reactions of cyclic and acyclic

1,3-dipoles with diphenylcyclopropenone and related compounds. A new rearrangement

AUTHOR(S): Matsukubo, Hiroshi; Kato, Hiroshi

CORPORATE SOURCE: Dep. Chem., Shinshu Univ., Matsumoto, Japan SOURCE: Journal of the Chemical Society, Chemical

Communications (1974), (10), 412-13

CODEN: JCCCAT; ISSN: 0022-4936 YPE: Journal

DOCUMENT TYPE: Journal LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Cycloaddn. of diphenylcyclopropenes, e.g. I, to mesoionic compds., e.g. II, occurred across the C:C double bond to give 33-63%

1,4-dihydrotetraphenylpyridine and tetraphenylthiopyran derivs. e.g. III. Cycloaddn. of PhCNO with I occurred across the C:O double bond to give, by

rearrangement, 40% triphenyl-1,3-oxazin-6-one. IT 54133-10-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 54133-10-7 CAPLUS

CN Propanedinitrile, 2-(1-methyl-2,3,5,6-tetraphenyl-4(1H)-pyridinylidene)(CA INDEX NAME)

OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)

ACCESSION NUMBER: 1974:133209 CAPLUS DOCUMENT NUMBER: 80:133209

ORIGINAL REFERENCE NO.: 80:21477a,21480a

TITLE: Synthesis and properties of heterofulvenes.

Derivatives of 2,6-dimethyl- γ -pyrone, $-\gamma$ -thiapyrone, and

N-butyl-2,6-dimethyl- γ -pyridone AUTHOR(S): Belsky, I.; Dodiuk, H.; Shvo, Y.

CORPORATE SOURCE: Dep. Chem., Tel-Aviv Univ., Tel-Aviv, Israel SOURCE: Journal of Organic Chemistry (1974), 39(7),

989-95

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal LANGUAGE: English

AB O-, S-, and N-containing heterofulvenes, derivs. of 2,6-dimethyl-γ-pyrone (I), -γ-thiapyrone (II), and

N-buty1-2,6-dimethy1-γ-pyridone were prepared The O and S

heterocycles were prepared by condensation of I and II, resp., with active methylene compds. in Ac20. The N heterocycles were obtained from the O heterocycles by reaction with BuNH2. Side reactions were observed when BuNH2 reacted with methyl 2,6-dimethyl-4H-pyran-4-ylidenenitroacetate and 2,6-dimethyl-4H-pyran-4-ylidenenitroacetone. A new convenient route to heterofulvenes which bear a single substituent at the exocyclic double bond was developed. Thus, heterofulvenes substituted by an acetyl group at the exocyclic double bond were found to undergo acetyl cleavage, under very mild acidic conditions, resulting in the formation of monosubstituted heterofulvenes. Deuterium exchange reactions in the systems under consideration were studied. The NMR, uv, and ir data of the disubstituted and monosubstituted heterofulvenes are discussed in terms of the heteroatom and the substituents at the exocyclic double bond.

IT 49810-95-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of) RN 49810-95-9 CAPLUS

CN Propanedinitrile, 2-(1-butyl-2,6-dimethyl-4(1H)-pyridinylidene)- (CA INDEX NAME)

OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

L5 ANSWER 34 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1971:463550 CAPLUS

DOCUMENT NUMBER: 75:63550
ORIGINAL REFERENCE NO.: 75:10067a,10070a

TITLE: Reactions of 4-dicyanomethylenepyrans with hindered

primary amines
AUTHOR(S): VanAllan, J. A.; Reynolds, G. A.

CORPORATE SOURCE: Res. Lab., Eastman Kodak Co., Rochester, NY, USA SOURCE: Journal of Heterocyclic Chemistry (1971),

8(3), 367-71

CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal

LANGUAGE: English

Reaction of 2,6-dimethyl- and 2,6-diphenyl-4-dicyanomethylene-4H-pyran with hindered primary amines such as isopropylamine and cyclohexylamine gave 1-alkyl-2-amino-3-cyano-6-methyl (or phenyl)-4-acetonylidene (or phenacylidene)-1,4-dihydropyridine derivs. 6-Methyl-4-acetonylidene examples underwent a facile thermal rearrangement to give 1-alkv1-2,6-dimethv1-4-dicvanomethvlene-1,4-dihvdropyridines. Several

reactions of the acylidene derivs. are described. 32883-35-5P 32883-36-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 32883-35-5 CAPLUS

CN Propanedinitrile, 2-[2,6-dimethyl-1-(1-methylethyl)-4(1H)-pyridinylidene]-(CA INDEX NAME)

32883-36-6 CAPLUS RN

CN Propanedinitrile, 2-(1-cyclohexyl-2,6-dimethyl-4(1H)-pyridinylidene)- (CA INDEX NAME)

OS.CITING REF COUNT: THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD 1 (1 CITINGS)

ANSWER 35 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1970:435253 CAPLUS

DOCUMENT NUMBER: 73:35253 ORIGINAL REFERENCE NO.: 73:5841a,5844a

TITLE: Reactions of some 4-methylene-4H-pyran derivatives

with primary and secondary amines

AUTHOR(S): Van Allan, James A.; Reynolds, George Arthur; Petropoulos, C. C.; Maier, D. P.

CORPORATE SOURCE: Res. Lab., Eastman Kodak Co., Rochester, NY, USA SOURCE:

Journal of Heterocyclic Chemistry (1970),

7(3), 495-507

CODEN: JHTCAD; ISSN: 0022-152X Journal

DOCUMENT TYPE:

LANGUAGE: English

OTHER SOURCE(S): CASREACT 73:35253

AB 4-Dicyanomethylene-4H-pyrans react with secondary amines to give

2-aminopyridine and 2-pyridone derivs., which, in turn, were used to prepare copyrine derivatives. These pyrans and pyrimary amines gave copyrine and iminopyridone derivatives in addition to dicyanomethylene-1, 4-dihydropyridines. Reaction of

cyanocarbamoylmethylene-4H-pyrans with secondary amines gave 2-pyrones, and with primary amines, gave copyrines and 1,4-dihydropyridine derivs.

RN 27337-89-9 CAPLUS

CN Propanedinitrile, 2-(1-methyl-2,6-diphenyl-4(1H)-pyridinylidene)- (CA INDEX NAME)

RN 27337-90-2 CAPLUS

CN Propanedinitrile, 2-(1-buty1-2,6-dipheny1-4(1H)-pyridinylidene)- (CA INDEX NAME)

RN 27368-13-4 CAPLUS

CN Propanedinitrile, 2-[2,6-diphenyl-1-(phenylmethyl)-4(1H)-pyridinylidene](CA INDEX NAME)

```
CH2-Ph
Ph
Ph
C-CN
```

OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)

L5 ANSWER 36 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN ACCESSION NUMBER: 1968:21803 CAPLUS DOCUMENT NUMBER: 68:21803 ORIGINAL REFERENCE NO.: 68:4183a,4186a TITLE: 4(1H)-Pyridylidene compounds. Synthesis and structure AUTHOR(S): Omote, Yoshimori; Kuo, Kung-Tu; Sugivama, Noboru CORPORATE SOURCE: Tokyo Kyoiku Univ., Tokyo, Japan SOURCE: Bulletin of the Chemical Society of Japan (1967), 40(7), 1695-7 CODEN: BCSJA8; ISSN: 0009-2673 DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 68:21803 GI For diagram(s), see printed CA Issue.

AB Compds. of the general formula I and anions of the general formula II are prepared Thus, dime 4-chloropyridine-2,6-dicarboxylate (III), m. 142°, is prepared The oil is removed from 1.5 g. 50% NaH dispersion, 10 ml. HCONMe2 added, the mixture cooled, 3.4 g. tert-BuOZCCH2CN slowly added, the mixture heated to 50°, a solution of 2 g. III in 10 ml. HCONMe2 slowly added, and the mixture heated 4.5 hrs. at 120° to give 1.5 g. tert-buyl \(\alpha \cdot \text{arg.} \) \(\alpha \cdot \text{corp.} \) \(\alpha

added,
and the mixture heated 30 min. to give I (R = CO2Et) (V), m. 149°
(BtOH). Similarly prepared is II (R = CN), m. 291°. A solution of V in
EtOH is treated with KOH (BtOH) to give II (R = CO2Et), m. 207-8°
(decomposition) (EtOH). N.M.R., ir, and uv data are given.
I 1679-16-3P 16833-89-16

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 16795-46-3 CAPLUS

CN 2,6-Pyridinedicarboxylic acid, 4-(dicyanomethylene)-1,4-dihydro-, 2,6-dimethyl ester (CA INDEX NAME)

RN 16833-89-9 CAPLUS

CN 2,6-Pyridinedicarboxylic acid, 4-(dicyanomethylene)-1,4-dihydro-, dimethyl ester, ion(1-) (8CI) (CA INDEX NAME)

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

ANSWER 37 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN 1967:508532 CAPLUS

ACCESSION NUMBER: DOCUMENT NUMBER: 67:108532

ORIGINAL REFERENCE NO.: 67:20455a,20458a

TITLE: Stable pyridine anhydro-bases AUTHOR(S): Boyd, Gerhard V.; Ezekiel, A. D.

CORPORATE SOURCE: Chelsea Coll. Sci. Technol., London, UK

SOURCE: Journal of the Chemical Society [Section] C: Organic

(1967), (19), 1866-8

CODEN: JSOOAX: ISSN: 0022-4952

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Twelve 2- and 4-methylenedihydropyridines containing strongly

electron-withdrawing groups on the methylene C atoms have been prepared One anomalous reaction was encountered. The anhydro-bases are protonated in acid solution (in 2 cases also in water) on the exocyclic C atom forming pyridinium ions.

16344-72-2P

16344-75-5P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

16344-72-2 CAPLUS RN

Propanedinitrile, 2-(1-methyl-4(1H)-pyridinylidene)- (CA INDEX NAME) CN

RN 16344-75-5 CAPLUS

CN Propanedinitrile, 2-(1,2,6-trimethyl-4(1H)-pyridinylidene)- (CA INDEX NAME)

DOCUMENT TYPE:

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L5 ANSWER 38 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1964:60896 CAPLUS DOCUMENT NUMBER: 60:60896

ORIGINAL REFERENCE NO.: 60:10678e-h,10679a-c

TITLE: Y-Pyrones. IV. Reactions with chelidonic acid. 2

AUTHOR(S): Eiden, F.; Peter, P.

CORPORATE SOURCE: Univ. Marburg/Lahn, Germany

SOURCE: Archiv der Pharmazie und Berichte der Deutschen

Pharmazeutischen Gesellschaft (1964), 297(1), 1-9

CODEN: APBDAJ: ISSN: 0376-0367

Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

of CA 58, 1455h. Chelidonic acid (I) di-Et ester and barbituric acid derivs. condense when heated in Ac20-AcOH to give pyranylidenebarbituric acids (CA 54, 247821). 1-Phenylchelidamic acid (II), the reaction product of I and PhNHZ, also reacted with reactive methylene compds. when heated in Ac20-AcOH with double decarboxylation to give 1-phenyl-1-azapyranylidene derivs. Active methylene compound and II (each (0.02 mole) in 20 ml. Ac20 and 5 ml. AcOH refluxed 3 hrs., the solution evaporated in vacuo (water pump), and the residue which solidified or became solid after addition of MeOH filtered gave the condensation product. The following compds. were prepared(Z = 1-phenyl-1-azapyran-4-ylidene throughout this abstract) [compound, % yield, m.p., \(\lambda \) (mm) (solvent given): III (R = R' = H, Y = O), 85, 325° (AcOH), 402 (dioxane); III (R = R' =

Me, Y = 0) (IIIa), 80, 310° (dioxane), 403-4 (dioxane); III (R = R' = H, Y = S), 50, 330° (AcOH), 430 (AcOH); IV, 79, 279°

(EtOH), 397 (MeOH); V, 63, 195° (70% EtOH), 430 (MeOH); VI, 49,

294° [HCONMe2 (DMF)], 476 (DMF); Z:C(CN)2, 64. 310° (DMF),375(AcOH); Z:C(CN)CO2Et, -, 182° (EtOH), 379 (MeOH); VII (R = R' = Me, R'' = H, R''' = CO2Et) (VIIa), 75,257° (EtOH), 401 (MeOH); VII (R = R' = H, R'' = R''' = CO2Et), 57, 249° (MeOH), 411 (MeOH); VII (R = R' = Me, R'' = R''' = CO2Et)(VIII), 79, 157-8° EtOH), 412 (MeOH); IX(R = H, R' = CO2Et),65, 170° (EtOH),378 (EtOH); IX (R = R' = CO2Et), 50, 139-40° (EtOH), 386 (MeOH). 1,3-Dimethylbarbituric acid heated with 1-phenyl-4(1H)-pyridone or 1,4-dihydro-4-oxo-1-phenylpicolinic acid (X) in Ac20-Ac0H gave IIIa, identical (m.p. and ultraviolet spectrum) with IIIa prepared above. VIIa (0.38 g.) in 20 ml. 80% H2SO4 heated 6 hrs. on a water bath, the solution cooled and poured over crushed ice, and the precipitate filtered off gave 0.23

VII (R = R' = Me, R'' = H, R''' = CO2H), m. .apprx.252° (rapid heating) (AcOH), λ (AcOH) 403 m μ , subliming on slow heating to give IIIa; p-bromophenacyl ester m. 267° (AcOH). VIII (0.96 g.) hydrolyzed with 80% H2SO4 as above gave 0.82 g. VII (R = R' = Me, R'' = R''' = CO2H), m. 236-7° (AcOH), λ (MeOH) 392 m μ . XI (R = Et) (E., loc. cit.) (0.7 g.) hydrolyzed with 80% H2SO4 as above gave 0.45 g. XI (R = H), m. above 320° (H2O), λ (DMF) 404 m μ . II (5.0 g.) suspended in 200 ml. EtOH and 50 ml. H2O refluxed 3 hrs. while introducing a vigorous stream of HCl, the resulting solution evaporated in vacuo

(water pump), and the sirupy residue heated 15 min. on a water bath in 25 ml. 2N HCl deposited 2.8 g. II mono-Et ester, m. 156° (decomposition) (iso-PrOH). II di-Et ester was prepared from II, EtOH, and HCl. 4-Oxo-4H-pyran-2-carboxylic acid (1.3 g.), 6.0 g. PhNH2, and 5.0 g. H2O refluxed 3 hrs., the solution cooled, the precipitate filtered off and dissolved in

hot H2O, and the solution treated with C and acidified gave 1.1 g. X, m. 189° (decomposition) (H2O), λ (H2O) 273 mμ; p-bromophenacyl ester m. 128° (45% EtOH).

94678-52-1

q.

(Derived from data in the 7th Collective Formula Index (1962-1966)) RN 94678-52-1 CAPLUS

CM 2,6-Pyridinedicarboxylic acid, 4-(dicyanomethylene)-1,4-dihydro-1-phenyl-, 2,6-diethyl ester (CA INDEX NAME)

93325-98-5P, Picolinic acid, 4-(dicvanomethylene)-1,4-dihydro-1-phenyl-, ethyl ester 93533-76-7P, Δ4(1H),α-Pyridinemalononitrile, 1-phenyl-RL: PREP (Preparation) (preparation of)

RN 93325-98-5 CAPLUS

CN 2-Pyridinecarboxylic acid, 4-(dicyanomethylene)-1,4-dihydro-1-phenyl-, ethyl ester (CA INDEX NAME)

RN 93533-76-7 CAPLUS

CN Propanedinitrile, 2-(1-phenyl-4(1H)-pyridinylidene)- (CA INDEX NAME)



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)

L5 ANSWER 39 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1964:60895 CAPLUS

DOCUMENT NUMBER: 60:60895

ORIGINAL REFERENCE NO.: 60:10678d-e

TITLE: Conversion of 4,1-benzoxazepine-2, 5(1H,3H)-diones

into 2-(α-hydroxyalkyl)-4-quinazolinones Uskokovic, M.; Iacobelli, J.; Toome, V.; Wenner, W.

AUTHOR(S): Uskokovic, M.; Iacobelli, J.; Toome, V
CORPORATE SOURCE: Hoffmann-La Roche, Inc., Nutley, NJ

SOURCE: Journal of Organic Chemistry (1964), 29(3),

582-4

CODEN: JOCEAH: ISSN: 0022-3263

DOCUMENT TYPE: Journal LANGUAGE: Unavaila

LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 60:60895

GI For diagram(s), see printed CA Issue.

AB $N-(\alpha-Haloacyl)$ -anthranilic acids are cyclized with HCONMe2 to

4,1-benzoxazepine-2,5(1H,3H)-diones (I), which in turn undergo ring

contraction to 2-(α -hydroxyalkyl)-4-quinazolinones (II or III) when

treated with NH3, primary amines, or N2H4.

IT 94678-52-1

(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 94678-52-1 CAPLUS

CN 2,6-Pyridinedicarboxylic acid, 4-(dicyanomethylene)-1,4-dihydro-1-phenyl-, 2,6-diethyl ester (CA INDEX NAME)

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EtO-C N C-OEt
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OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

L5 ANSWER 40 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN ACCESSION NUMBER: 1963:66941 CAPLUS

DOCUMENT NUMBER: 58:66941
ORIGINAL REFERENCE NO.: 58:11496h,11497a-d

TITLE: Alkyl substituted pyrylo- and pyridinocyanines. I.
2,6-Dimethylovrylo- and 2,6-dimethylovridinocyanine

from 2,6-dimethyl-γ-pyrone
AUTHOR(S): Kelemen, Jozsef: Wizinger, Robert

CORPORATE SOURCE: Univ. Basel, Switz.

SOURCE: Helvetica Chimica Acta (1962), 45, 1908-17

CODEN: HCACAV; ISSN: 0018-019X

DOCUMENT TYPE: Journal LANGUAGE: German

GI For diagram(s), see printed CA Issue.

2,6-Dimethyl-y-pyrone was condensed with active methylene and methyl compds. by the procedure of Woods (CA 52, 128531) to give the cyanine dyes I or II, which were condensed with MeNH2 in EtOH to give the pyridine derivs. III or IV. Thus, to a hot saturated solution of I [R = (NC)2C]

(Woods,

loc. cit.) in EtOH was added an excess of MeNH2 in EtOH, the mixture refluxed 30 min., cooled, and the precipitate washed with ice-cold EtOH to give III [R = (NC)2C], m. 225-8°, colorless in EtOH, λmaximum 356 mu. Similarly were prepared (compound, R, m.p., color in EtOH, Amaximum in mu; m.p., color in EtOH, and Amaximum in mu of pyridine analogs given): I, p-O2NC6H4C(CN), 205-6°, yellow, 398, 224-6°, red, 487; I, 1,3-indandione-2-ylidene, 258-60° pale yellow, 404,303-4°, pale yellow, 387; I, 3-methyl-1-phenyl-5-pyrazolon-4-ylidene, 212-13°, orange, 410, 280-3°, yellow, 384; I, 3-(1,3-indandion-2-ylidene)-1-indanone-2ylidene, 255-60° (decomposition), violet, 412 and 568, 313-14°, blue-violet, 558; II, 3-methyl-2-benzoxazolinylium, above 260° (decomposition), yellow, 414 and 430, above 300°, pale yellow, 412; II, 3-methyl-2-henzothiazolinylium, 296° (decomposition) (BF4- salt decompose 274°), yellow, 436 and 460 (BF4- salt 436 and 460), 328-9°, yellow, 440; II, 1-methyl-2(1H)-quinolylium, 220-4° (decomposition), yellow, 482, 258-9°, orange, 479 and 503; II, 1-methyl-4(1H)-quinolylium, 213-15° (decomposition), orange, 508, 237°, violet, 528; II, 2,6-diphenyl-4-pyrylium 223-4°, blue-red, 512, 243-4°, yellow, 454; and II, 4,6-diphenyl-2-pyrylium, 212-13° (HO2CCH2SO3H salt m. 198-200°), red-violet, 540 and 566 (HO2CCH2SO3H salt 540 and 566), 245°, carmine red, 495. Also prepared was the yellow N-phenyl analog of III (R = 3-methy1-2-benzothiazolylium) m. >250° (decomposition), Amaximum 452 mμ. 1,3,3-Trimethyl-2-(N-hydroxyformimidoyl)-2indolinylium perchlorate (3 g.), 2.8 g.

2,6-diisopropyl-4-methyl-4-pyrylium perchlorate, and 0.8 g. fused powdered

NaOAc in 20 ml. HOAc was boiled 1 min., the mixture cooled, and poured into Et20 to give (1,3,3-trimethyl-2-indolenine)-(2,6-

diisopropylpyrylo)monomethinecvanine perchlorate, m. 178.

4664-22-6

(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 4664-22-6 CAPLUS

CN Propanedinitrile, 2-(4(1H)-pyridinylidene)- (CA INDEX NAME)

16344-75-5, Δ4(1H),α-Pyridinemalononitrile, 1,2,6-trimethvl-

(spectrum of) RN 16344-75-5 CAPLUS

CN Propanedinitrile, 2-(1,2,6-trimethyl-4(1H)-pyridinylidene)- (CA INDEX

OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD (7 CITINGS)

L5 ANSWER 41 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1963:66940 CAPLUS DOCUMENT NUMBER:

58:66940

ORIGINAL REFERENCE NO.: 58:11495g-h,11496a-h

TITLE: Derivatives of imidazobenzothiadiazole,

imidazobenzoselenadiazole, imidazobenzotriazole, and

imidazoquinoxaline

AUTHOR(S): Fridman, S. G.; Kotova, L. I.

CORPORATE SOURCE: Inst. Org. Chem., Kiev

Zhurnal Obshchei Khimii (1962), 32, 2871-82 SOURCE:

CODEN: ZOKHA4; ISSN: 0044-460X

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

cf. CA 55, 24728e; 58, 1564c. Dyes based on the title heterocyclic

systems have their absorption maximum shifted considerably toward longer wavelengths in comparison with imidocarbocyanines.

2-Methyl-5,6-dinitrobenzimidazole di-HCl treated with Me2SO4 in aqueous MeOH-NaOH at 90-5° gave 90% 1,2-dimethyl-5,6-dinitrobenzimidazole, m. 239-40% which with Sn-HCl gave 1,2-dimethyl-5,6-diaminobenzimidazole

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(I) (61%), m. 278°. This with SOC12 in pyridine-C6H6 at reflux 5
hrs. gave 78% 1,2-dimethylimidazo[4,5-f]-2,-1,3-benzothiadiazole, m.
182°; the yield was 54% when C6H6 was omitted and the reaction run
2 hrs. in refluxing pyridine; the base formed the Me perchlorate,
colorless needles, after treatment with p-MeC6H4SO3Me, followed by NaClO4.
2-Methyl-5,6-diaminobenzimidazole (II) and H2SeO3 in H2O gave 61% yellow
2-methylimidazole [4,5-f]-2,1,3-benzoselenadiazole-HCl, decomposed
310°; free base m. 275-6°. Similarly was prepared the
1,2-di-Me analog, vellow needles, m. 243° also formed from the 2-Me
analog and Me2SO4 in 10% NaOH. The base formed a methiodide, m.
291°. 2-Methyl-and 1,2-dimethylimidazo[4,5-f]benzotriazole bis(Et
perchlorate) and bis(Me perchlorate), m. 266-7°, were prepared from
the resp. bases (Kym and Ratner, CA 7, 1184; Fries, Ann. 454, 219(1927)).
Treatment of I in 2M AcOH-4M NaOAc with glyoxal-NaHSO3 at 60° for 1
hr. gave after addition of NaOH and K2CO3 57% yellow
1,2-dimethylimidazo[4,5-g]quinoxaline, m. 214°; Me perchlorate, a
solid. I refluxed with Ac2 in MeOH 3 hrs. gave 75%
1,2,6,7-tetra-methylimidazo[4,5-q]quinoxaline, m. 318°; methiodide
m. 275°. II-HCl and benzil in aqueous EtOH gave 60% yellow
2-methyl-6, 7-diphenylimidazo[4,5-q]quinoxaline, m. 285-6° which
with Me2SO4 in NaOH gave 76% 1,2-dimethyl analog, m. 221°, also
formed from 1,2-dimethyl-5,6-diaminobenzimidazole and benzil in EtOH; the
base formed an ethiodide, m. 291-2°. Similar reaction with
phenanthrenequinone gave 557% 1,2-dimethylimidazo-[4,5-q]phenanthro[9,10-
b]quinoxaline, m. 282°. Acenaphthenequinone similarly gave 88%
1,2-dimethylimidazo [4,5-g] acenaphtheno[1,2-b]quinoxaline, m.
310°. Heating the appropriate methiodides or Me tosylates with
HC(OEt)3 in PhNO2 1 hr. at 150-60° gave the following dyes (%
yield, m.p., and λmaximum in mμ given): bis [1,3-dimethylimidazo
[4,5-f] -2,1,3-benzothiadiazole-2]trimethinecyanine iodide, 42,
286°, 576; bis[1,3-dimethylimidazo[4,5-f]-2,1,3-benzoselenadiazole-
2]trimethinecyanine p-toluenesulfonate, 79,320°, 596;
bis[1,3,5,7-tetramethylimidazo-[4,5-f]benzotriazole-2]trimethinecyanine
triperchlorate, 58, 323° 568;
bis[1,3-dimethylimidazo[4,5-g]quinoxaline-2] trimethinecyanine iodide, --,
--, 560; bis[1,3,6,7-tetramethylimidazo[4,5-g]quinoxaline-
2]trimethinecyanine iodide, 61, 290-1°, 556; and bis
[1-methyl-3-ethyl-6,7-diphenylimidazo [4,5-q]
quinoxaline-2|trimethinecyanine iodide, 55, >320° 594. Similar
condensations with 2-(B-acetanilidovinyl)benzothiazole or
a-naphthothiazole ethiodide in Ac20-Et3N gave the following dves
(same data given): [1,3-dimethylimidazo[4,5-f]-2,1,3-benzothiadiazole-2]-
[3-ethylbenzothiazole-2]trimethinecyanine iodide, 23, 247° 564;
[1,3-dimethylimidazo[4,5-f]-2,1,3-benzoselenadiazole-2]
[3-ethylbenzothiazole-2][trimethinecyanine iodide, 36, 281° 576;
[1,3-dimethylimidazo[4,5-f]-2,1,3-benzothiadiazole-2]
[3-ethylnaphtho[2,1-d] thiazole-2]trimethinecvanine iodide, 41,
280°, [585; [1,3-dimethylimidazo[4,5-f]-2,1,3-benzoselenadiazole-
2] [3- ethylnaphtho[2,1-d]thiazole-2]trimethinecyanine
p-toluenesul-fonate, 42, 284-5°, 594;
[1,3,5,7-tetramethylimidazo[4,5-f]-benzotriazole-2]
[3-ethylbenzothiazole-2] trimethinecyanine iodide, 52,211-12°, 560;
[1,3-dimethylimidazo[4,5-g]quinoxaline-2][3-ethylbenzothiazole-
2]trimethinecyanine iodide, 46, 273° 552;
[1,3,6,7-tetramethylimidazo [4,5-g] quinoxazoline-2]
[3-eth-ylbenzothiazole-2]trimethinecyanine iodide, 33, 320°, 547;
[1-methyl-3-ethyl-6,7-diphenylimidazo[4,5-q]quinoxaline-2-] -
[3-ethylbenzothiazole-2]trimethinecyanine iodide, 51, 291°, 566.
Similarly, appropriate methiodides or Me p-toluenesulfonates treated with
2-(β-acetanilidomethylene)-N-ethylrhodanine in EtOH-Et3N gave the
following dyes (same data given): 3-ethyl-5-[1,3-dimethylimidazo
[4,5-f]-2,1,3-benzothiadiazole-2-ethylidene]thiazolidine-2-thione-4-one,
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64, 324°, 533; 3-ethyl-5-[1,3-dimethylimidazo [4,5-f] -
     2,1,3-benzoselenadiazole-2-ethyli-denelthiazolidine-2-thione-4-one, 22,
     320°, 564; 3-ethv1-5-[1,3,5,7-tetramethylimidazo [4,5-f]
     benzotriazole-2-ethvlidenel-thiazolidine-2-thione-4-one Me
     p-toluenesulfonate, 32, 272-3°, 547; 3-ethyl-5-[1,3-dimethylimidazo
     [4,5-q] quinoxaline-2-ethyli-dene]thiazolidine-2-thione-4-one, 70,
     >300°, 544; 3-ethyl-5-[1,3,6, 7-tetramethylimidazo [4,5-q]
     quinoxaline-2-ethylidene| -thiazolidine-2-thione-4-one, 53, >300°,
     540; 3-ethvl-5-[1-methvl-3-ethvl-6,7-diphenvlimidazo[4,5-q]
     guinoxaline-2-ethylidenel-thiazolidine-2-thione-4-one, 55, >310°,
     558. Heating the appropriate methiodides with 2-(methylthio)benzothiazole
     ethiodide in EtOH-Et3N gave the following dyes (same data
     given): [1,3-dimethylimidazo[4,5-g]guinoxaline2]
     [3-ethylbenzothiazole-2]monomethinecyanine perchlorate, 39, --, 441;
     [1,3,6,7-tetramethylimidazo[4,5-g]quinoxaline-2]
     [3-ethylbenzothiazole-2]monomethinecyanine iodide, 25, 206°, 436;
     and [1-methyl-3-ethyl-6,7-diphenylimidazo[4,5-g] quinoxaline-2]
     [3-ethylbenzothiazole-2]monomethinecyanine iodide, 40, 271-2°, 458.
     The propriate Me p-toluenesulfonates and p-Me2NC6H4CHO in Ac2O gave (same
     data given): 2-[p-dimethylaminostyryl]-1-methylimidazo[4,5-f]-2,1,3-
     benzothiadiazole methiodide, 76, 273°, 503;
     2-(p-dimethylaminostyryl)-1-methylimidazo[4,5-f]-2,1,3-benzoselenadiazole
     Me p-toluenesulfonate, 72,272-3°, 519;2-(p-dimethylaminostyryl)-
     1.5.7-trimethylimidazo[4.5-f]benzo-triazole dimethiodide, 35, 301°,
     517. The last dye tended to lose its iodine content on repeated
crystallization
     from H2O.
     4664-22-6
        (Derived from data in the 7th Collective Formula Index (1962-1966))
     4664-22-6 CAPLUS
     Propanedinitrile, 2-(4(1H)-pyridinylidene)- (CA INDEX NAME)
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RN

CN

ACCESSION NUMBER: 1961:144162 CAPLUS DOCUMENT NUMBER: 55:144162 ORIGINAL REFERENCE NO.: 55:27301d-h TITLE: 1-Alkyl-2(1H)-pyridone derivatives. IV. 1-Phenethyl-3-substituted-2(1H)-pyridones AUTHOR(S): Tomisawa, Hiroshi; Agatsuma, Tomie; Kamura, Yuichi Yakugaku Zasshi (1961), 81, 947-50 SOURCE: CODEN: YKKZAJ: ISSN: 0031-6903 DOCUMENT TYPE: Journal LANGUAGE: Unavailable

L5 ANSWER 42 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

cf. CA 54, 3416g. 1-Phenethyl-3-cyano-2(1H)-pyridone (I) (15.3 g.) in 10 g. KOH, 10 ml. H2O, and 150 ml. EtOH refluxed 5 hrs., the solution concentrated in vacuo, 200 ml. H2O added, the solution filtered with C, and the filtrate

treated with HCl gave 14 g. 1-phenethyl-3-carboxy-2(1H)-pyridone (II), needles, m. 161-3°. Catalytic reduction of II with Raney Ni gave a

quant. yield of 1-phenethyl-3-carboxy-2-piperidone (III), prisms, m. 98-9° (EtOH). III in AcOH refluxed 2 hrs., the AcOH removed, and the product treated as usual gave 1-phenethyl-2-piperidone, oil. II (18.7 g.), 2 ml. HCONNe2, and 52 ml. SCOL2 refluxed 2 hrs., 100 ml. BtOH added portionwise, the mixture refluxed 1 hr., and the product treated as usual gave 18 g. 1-phenethyl-3-carbethoxy-2(1H)-pyridone (IV), oil, b0.015 191°. IV (7.3 g.) and 2 moles N2H4.HZO with a small amount of EtOH refluxed 3 hrs. and the solvent removed gave 5.7 g.
1-phenethyl-3-hydrazinocarbonyl-2(1H)-pyridone-HCl (V), m. 88-9.5° (10% HCl). V (2 g.) in 50 ml. 5% HCl at 0° treated dropwise with a concentrated solution containing 0.5 g. NaNO2, C6H6 added, the excess HNO3

decomposed

with urea, the C6H6 layer and 1 mole PhCH2OH refluxed 3 hrs., and the solvent removed gave 1.4 g. 1-phenethyl-3-benzyloxycarbonylamino-2(IH)-pyridone (VI), oil. VI (1.6 g.), 10 ml. Ac2O, and 10 ml. concentrated HCl refluxed 4 hrs. and the product treated as usual gave 0.48 g. 1-phenethyl-3-amino-2(IH)-pyridone-HCl (VII); Ac derivative, leaves, m. 92-3°. VII (0.3 g.) in 10 ml. concentrated HCl at 0° treated with 0.1 g. NaNO2 and the product treated as usual gave 0.22 g. 1-phenethyl-3-chloro-2(IH)-pyridone (VIII), columns, m. 129-30°. Similarly, 0.3 g. VII and 10 ml. 47% HBr gave 75% 3-Br analog of VIII, m. 139-40°; 3-iodo analog of VIII, m. 115-16°; 3-NO2 analog of VIII, m. 150-1°. VII (0.2 g.) in 2 ml. concentrated H2SO4 and 5 ml. H2O at 0° treated with 0.1 g. NaNO2, this added into Cu2(CN)2 solution (ffrom 7 g. CuSO4.5H2O and 7.5 g. KCN), kept overnight, and the product extracted with CHCl3 gave 0.1 g. 1, bo.02 175-90°, m. 115-16°.

IT 102654-01-3P, Δ4(1H),α-Pyridinemalononitrile,

2,6-dimethyl- 107151-81-5P, Δ4(1H),α-Pyridinemalononitrile,

1-benzylideneamino-2,6-dimethyl-

RL: PREP (Preparation) (preparation of)

RN 102654-01-3 CAPLUS

CN Propanedinitrile, 2-(2,6-dimethyl-4(1H)-pyridinylidene)- (CA INDEX NAME)

RN 107151-81-5 CAPLUS

CN Propanedinitrile, 2-[2,6-dimethyl-1-[(phenylmethylene)amino]-4(1H)pyridinylidene]- (CA INDEX NAME)

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N CH-Ph
Me
N Me
C-CN
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CN

INDEX NAME)

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L5 ANSWER 43 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER:
                         1961:144161 CAPLUS
DOCUMENT NUMBER:
                         55 - 144161
ORIGINAL REFERENCE NO.:
                        55:27301b-d
TITLE:
                         Non-benzenoid aromatic heterocycles. III. Conversion
                         of 4-pyrone derivatives into 4-pyridone derivatives
                         Kato, Hiroshi; Ogawa, Takatoshi; Ohta, Masaki
AUTHOR(S):
CORPORATE SOURCE:
                         Tokvo Inst. Technol
SOURCE:
                         Bulletin of the Chemical Society of Japan (
                         1960), 33, 1468-9
                         CODEN: BCSJA8: ISSN: 0009-2673
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         Unavailable
    4-Pyrones reacted with amines to give 4-pyridones.
     4-(Dicyanomethylene)-2.6-dimethyl-4H-pyran (I) (3.5 g.) and 4 g. PhNH2
     refluxed 1 hr. and the mixture washed with dilute HCl gave 20%
     N-phenyl-4-(dicyanomethylene)-2,6-dimethyl-1,4-dihydropyridine, m.
     314-15° (HOAc). Similarly, I with BzNH2 at 150° gave 34%
     N-benzyl-4-(dicyanomethylene)-2,6-dimethyl-1,4-dihydropyridine, m.
     242-5° (EtOH), and with NH2NH2.H2O at 100° gave 40%
     N-amino-4-(dicyanomethylene)-2,6-dimethyl-1,4-dihydropyridine, m.
     291-2° (decomposition) (HOAc). 4-(Ethoxycarbonylcyanomethylene)-2,6-
     dimethyl-4H-pyran with BzNH2 gave N-benzyl-4-
     (ethoxycarbonylcyanomethylene) -2,6-dimethyl-1,4-dihydropyridine, m.
     183-4° (EtOH), with NH2NH2.H2O gave
     N-amino-4-(ethoxycarbonylcyanomethylene)-2,6-dimethyl-1,4-dihydropyridine,
    m. 217-18° (EtOH), but did not react with PhNH2 or HCONH2.
     N-Amino-4-(dicvanomethylene)-2,6-dimethyl-1,4-dihydropyridine (0.6 g.) and
     0.4 g. BzH refluxed 1 hr. gave 0.6 g. (crude)
     N-benzalamino-4-(dicyanomethylene)-2,6-dimethyl-1,4-dihydropyridine, m.
     294-5° (AcOH). I (5 g.) in 5 g. HCONH2 kept 1 hr. at 150°
     gave 1.7 g. 4-(dicyanomethylene)-2,6-dimethyl-1,4-dihydropyridine, m.
     330-1° (HCO2H).
    62071-85-6P, Δ4(1H), α-Pyridinemalononitrile,
     1-amino-2,6-dimethvl-
                             102654-01-3P.
     Δ4(1H), α-Pyridinemalononitrile, 2,6-dimethyl-
     106883-97-0P, Δ4(1H), α-Pyridinemalononitrile,
     2,6-dimethyl-1-phenyl-
                             107151-81-5P,
     \Delta 4 (1H), \alpha-Pvridinemalononitrile,
     1-benzylideneamino-2,6-dimethyl-
                                       107518-55-8P.
     Δ4(1H), α-Pyridinemalononitrile, 1-benzyl-2,6-dimethyl-
     RL: PREP (Preparation)
        (preparation of)
RN
    62071-85-6 CAPLUS
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Propanedinitrile, 2-(1-amino-2,6-dimethyl-4(1H)-pyridinylidene)- (CA

- RN 102654-01-3 CAPLUS
- CN Propanedinitrile, 2-(2,6-dimethyl-4(1H)-pyridinylidene)- (CA INDEX NAME)

- RN 106883-97-0 CAPLUS
- CN Propanedinitrile, 2-(2,6-dimethyl-1-phenyl-4(1H)-pyridinylidene)- (CA INDEX NAME)

- RN 107151-81-5 CAPLUS
- CN Propanedinitrile, 2-[2,6-dimethyl-1-[(phenylmethylene)amino]-4(1H)pyridinylidene]- (CA INDEX NAME)

OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

L5 ANSWER 44 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1961:81717 CAPLUS

DOCUMENT NUMBER: 55:81717
ORIGINAL REFERENCE NO.: 55:15482c-e

TITLE: Conversion of 4-pyrone derivatives into 4-pyridone

derivatives
AUTHOR(S): Kato, Hiroshi: Oga

AUTHOR(S): Kato, Hiroshi; Ogawa, Takatoshi; Ohta, Masaki CORPORATE SOURCE: Tokyo Inst. Technol., Japan

SOURCE: Chemistry & Industry (London, United Kingdom) (

1960) 1300 CODEN: CHINAG: ISSN: 0009-3068

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.
AB O.CMe:CH.C[:C(CN)R].CH:CMe2 (I) (R = CN) (Ia) with PhNH2 gave 20%

R'N.CMe:CH.C[:C-(CN)R].CH.CMe (II) (R = CN, R' = Ph), m. 314-15°. Similarly prepared were II (R = CN, R' = PhCH2), m. 242-5°, with PhCH2NH2 (III), and II (R = CN, R' = NH2) (IV), m. 291-2°, with NZH4.HZO (V). The structure of IV was established by conversion to its benzal derivative, m. 254-5°. Heating Ia in HCONH2 gave II (R = CN, R')

= H) or 34% 2,6-dimethyl-4-dicyanomethylpyridine, m. 294-5°. I (R = CO2Et) with III gave 80% II (R = CO2Et, R' = PhCH2), m. 183-4°, and with V gave 71% II (R = CO2Et, R' = NH2), m. 217-18°.

TT 62071-85-6P, Δ4(1H),α-Pyridinemalononitrile,

1-amino-2,6-dimethyl- 102654-01-3P, $\Delta 4 \text{(1H)}, \alpha$ -Pyridinemalononitrile, 2,6-dimethyl-

106883-97-0P, $\Delta 4$ (1H), α -Pyridinemalononitrile,

2,6-dimethyl-1-phenyl- 107151-81-5P,

Δ4(1H),α-Pyridinemalononitrile, 1-benzylideneamino-2,6-dimethyl-

1-benzylideneamino-2,6-dimethyl- 107518-55-8P, $\Delta 4 (1H), \alpha$ -Pyridinemalononitrile, 1-benzyl-2,6-dimethyl-

RL: PREP (Preparation) (preparation of)

RN 62071-85-6 CAPLUS

CN Propanedinitrile, 2-(1-amino-2,6-dimethyl-4(1H)-pyridinylidene)- (CA INDEX NAME)

- RN 102654-01-3 CAPLUS
- CN Propanedinitrile, 2-(2,6-dimethyl-4(1H)-pyridinylidene)- (CA INDEX NAME)

- RN 106883-97-0 CAPLUS
- CN Propanedinitrile, 2-(2,6-dimethyl-1-phenyl-4(1H)-pyridinylidene)- (CA INDEX NAME)

- RN 107151-81-5 CAPLUS
- CN Propanedinitrile, 2-[2,6-dimethyl-1-[(phenylmethylene)amino]-4(1H)pyridinylidene]- (CA INDEX NAME)

107518-55-8 CAPLUS

CN Propanedinitrile, 2-[2,6-dimethyl-1-(phenylmethyl)-4(1H)-pyridinylidene]-(CA INDEX NAME)

RN

L5 ANSWER 45 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1957:43354 CAPLUS

DOCUMENT NUMBER: 51:43354

ORIGINAL REFERENCE NO.: 51:8096e-i,8097a-i,8098a-f

TITLE: Pseudo bases. I. Additions of methyl and methylene

ketones to pyridinium salts

AUTHOR(S): Krohnke, Fritz; Ellegast, Konrad; Bertram, Ewald CORPORATE SOURCE: Forschungsinst. Dr. A. Wander, A.-G., Sackingen/Baden,

Germany

SOURCE: Justus Liebigs Annalen der Chemie (1956),

600, 176-98 CODEN: JLACBF: ISSN: 0075-4617

DOCUMENT TYPE: LANGUAGE: Journal Unavailable

197°; 90% 3-NC, m. 187-8°; and 96% 3-AcNH, m. 231°.

GI For diagram(s), see printed CA Issue.

AB Pyridinium, quinolinium, and isoquinolinium bases form addition compds. with simple Me ketones and with certain methylene ketones. The adducts are easily retrograded by acids, and can be dehydrogenated to form bases that yield stable salts. The adducts are considered to be "salts" in which the organic cation and anion are stabilized with regard to resonance, and which are related to bases (termed mesomeric cations) which are considered intermediate between ammonium arid carbinol bases. The possibility of existence, of pseudo bases (i.e. carbinol bases) increases with decreasing aromaticity of the heterocycle. With hyperaromatic N-heterocycles like pyridine, such bases could not be isolated. In the case of quinoline and isoquinoline derivs., in certain instances such bases could be prepared, but the formation of mesomeric cations was favored. In the acridine series, and with heterocycles containing O, carbinol bases are favored over ammonium or mesomeric cations; this also occurs in the Ph3CH series. Hydrogenation of heterecycles greatly increases the stability of the carbinol bases, which are easily isolated. 2,6-C12C2H2Me (322 g.) in 400 cc. CC14, stirred and irradiated was treated dropwise with 100.2 cc. Br in 50 cc. CC14 giving 422 g. 2,6-C14C4H4CH4Br (I), m. 55°; details of purification are given. I is a powerful lacrimator. I with a slight excess of pyridine (cf. C.A. 47, 1704f), heated in Me2CO gave, in excellent yield, N-(2,6dichlorobenzyl)pyridinium bromide (II) m. 216-17°; this in MeOH with p-ONC6H4NMe6 (IIa) gave 58% 2,6-Cl6C6H6CH:N→O) C6H6NMe6-4 (III), yellow prismatic spikes, m. 152-3°. When 10% pyridine or α -picoline was added to the MeOH, 75% and 81% III, resp., were obtained. Formed similarly from I and appropriately substituted pyridines were the following derivs. of II: 93% 3-Me, m. 183-4° (from 1:1 EtOH-Et20); 89% 3-HOCH2.H2O, m. 111-13°; 97% 3-H2NCO (IIIa), m. 246-8°; 95% 3-Et2-NCO, m.

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II (1.92 g.) in 15 cc. Me2CO and 3 cc. H2O at 20° with 5 cc. 2N
NaOH gave 1.69 g. Me2CO adduct, C2H2ONC12 (IV), colorless rhombs, m.
94-5° (when cooled to 0°; not recrystallizable), forming a
brown resin on standing. Similarly formed were the following adducts of
II, analogs of IV; 58% BzMe (IVa), pale yellow prisms, m. 80-1°;
70% cyclohexanone, yellowish leaflets, m. 83-4°; 66% deoxybenzoin,
yellow, m. 87-8°; and 79% monohydrate of the 3-H2NCO derivative of IV,
m. 138-9° (decomposition). In the following dehydro compds. R: =
N-[2,6-dichlorobenzyl]-1,4-dihydro-4-pyridylidene. To 6.38 g. II in 25
cc. MeOH, 5 cc. BzMe, and 1.8 g. IIa at 20° under N was added 20
cc. 2N NaOH, giving, after 4 hrs. 5.4 g. R:CHBz (IVb), dark vellow rhombs,
m. 166-7° (HC104 salt, leaflets, m. 216-17°; HBr salt, thin
rhombs, m. 187-88°). Similarly formed were the following compds.
(reaction time in hrs., % yield, crystalline color and form, and m.p. given):
R: CHAc (IVc), 3, 97, yellow needles changing to octahedra, 203-4°
(HC104 salt colorless, m. 192-3°); R:CHCOEt, 1.5, 19, yellow
prisms, 219-20°; R:CHCOC6H4Me-4, 7, 70, yellow needles,
213-14°; R:CHCOC6H4OMe-4, 21, 72.6, yellow needles,
199-200°; R:CHCOC6H4Br-4, 7, 59.8, yellow prisms, 218-19°;
R:C. CH2.CH2.CH2.CO, 4, 60, yellow rectangles with violet luster,
229-30°; R: C.CO.CH2.CH2.CH2.CH2, 2, 98.5, yellow prisms,
209-10°; R: C. CO. CH2.CHMe.CH2.CH2, 2.5, 90, orange polyhedrons,
207-8° (resinifying on storage); R:C.CO.CH2.CH2.CHMe.CH2, 2, 77.8,
yellow triboelectric needles, 186°; R:C.CH2.CH2.CH2.CH2.CH2.CO, 20,
46, yellow prisms, 167-8°; R: CH-NO2, 2, 14.8, yellowish brown
leaflets with blue luster, 233-5° (sintering at 230°). The
following were prepared using aeration (instead of IIa) and 2N MeONa in
place of aqueous NaOH: R:C(CN)2, 24, 30, colorless needles, 234-5°;
cyclopentadienylidene analog, 40, 51°, red prisms with blue luster,
199-20° (from HCONMe2); 1-indenylidene analog (V), 30, 23, red
microprisms with steely luster, 234-5° (from C6H6). The
9-fluorenylidene analog of V, C25H17NCl2, dark red prisms with blue
luster, m. 232-3°, when formed with IIa, 55.7% yield in 90 hrs.,
with air, 10% in 96 hrs. Using air as oxidant, 0.64 g. II, 0.3 g.
1,3-indandione in 10 cc. MeOH containing 0.4 cc. 10N NaOH gave, after 24 hrs.,
0.32 g. N-[2,6-dichlorobenzyl]-4-[1,3-dioxo-2-hydrindylidene]-1,4-
dihydropyridine, C12H13O2NC12, yellow, m. 334-5° (from AcOH).
Similarly, II and 1-phenyl-3-methyl-5-pyrazolone gave 70%
N-[2,6-dichlorobenzyl]-4-[1-phenyl-3-methyl-5-pyrazolon-4-ylidene]-1,4-
dihydropyridine, yellow, m. 223-4°. The following compds.,
R'N.CH:CH2C(:CHR'').CR''':-CH, formed by dehydrogenation (with IIa) of the
appropriate ketone adducts (R' = 2,6-Cl2C6H3CH2; R''',R'', reaction time,
% yield, crystalline properties, and m.ps. given): Me, Ac, 3, 89, yellow
rhombs, 193° (HClO4 salt, m. 190-1°; HBr salt, hexagons, m.
216-18°); CH2OH, Ac, 1.5, 95.6, yellow hexagons, 205-6°;
CH2OH, Bz, 17, 65, yellow rhombs, 207° (decomposition) (HBr salt,
yellow, m. 220-1°, yellowish green ultraviolet fluorescence); CONH2
Ac, 1.5, 97.6, yellow, 220-1° (HBr salt, decompose 289°);
CONH2, Bz, 3, 89, -, -(HCl salt, yellow rhombic leaflets, 271-2°); CONH2, p-MeOC6H4CO, 72, 85, yellow, 278-9° (HCl salt, orange
prisms, 271-2°, blue ultraviolet fluorescence in H2O); CONEt2, Bz, 7.97, yellow, 201°; CONEt2 Ac, 5.5, 86.5, yellow hexagons,
170-1° (when crude, m.p. lower on recrystn.); CONH2, (:CHR'' =)
2-cyclohexanonylidene, 7, 71.4, yellow rectangles, m. 201-2° (decomposition). The 3,4-Cl2 isomer of II (0.96 g.) in 10 cc. Me2CO and 10 cc.
H2O at 20° was shaken with 0.6 cc. 10N NaOH, 20 cc. Me2CO added to
dissolve the resin, and then 0.63 g. KMnO4 in 10 cc. Me2CO. The warmed
mixture was filtered, treated with C, refiltered, H2O added to incipient
cloudiness and cooled to 0° giving 0.32 g.
N-[3,4-dichlorobenzyl]-4-acetonylidene-1,4-dihydropyridine (VI), yellow,
m. 146-7° (from 1:1 C6H6-ligroine). Similarly formed were the
2,4-dichloro isomer of VI, yellow, m. 144-5° and the 4-monochloro
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analog of VI, yellow, m. 133-4° (from Et20). VI and its isomer and
analog resinify on standing. Oxidation of IVa in pyridine, with KMnO4
gave IVb. Formed similarly was the 3,4-dichloro isomer of IVb, yellow, m.
166° (cf. Baker and McEvoy, C.A. 50, 3454g). In place of IIa, K
nitrosodisulfonate converted IV into 77% IVc. IV (0.62 g.) in dry C6H6
with 0.22 g. benzoquinone in 20 min. formed 0.75 g. adduct
IVc.1,4-C6H4(OH)2, orange prisms, m. 176-8°, also formed from IVc
and 1,4-C6H4(OH)2, readily reconverted into IVc by treatment with HClO4
followed by treatment with 2N NaOH. In the following cases adducts of
N-phenethylpyridinium bromide (VII) were not isolated but dehydrogenated
directly. E.g., 2.64 g. VII with 0.8 g. IIa and 3 cc. BzMe in 15 cc. MeOH
under N. with 2 cc. 10N NaOH gave 1,6 q.
N-phenethyl-4-phenylidene-1,4-dihydropyridine, yellow hexagons, m.
198-9° (from 50% MeOH, the mother liquor from which gave 0.05 g.
azoxydimethylaniline, orange, m. 241-2°). Similarly prepared from
Me2CO was the 4-acetonylidene analog, yellow rectangles, m. 187-8°.
Formed from the appropriate pyridinium salts, sometimes under slightly
modified conditions were the following
4-acetonylidene-1,4-dihydropyridines: 45% N-PhCH(OH)CH2, yellow rhombs,
decompose about 227-8°; 72% N-[4-C1C6H4CH2CH2], yellow leaflets, m.
193-4°; 34.3% N-[4-C1C6H4CH(OH)CH2], vellow rhombs, m.
230-1° (decomposition); 42% N-[4-O2NC6H4CH(OH)CH2], slender yellow
leaflets, decompose 220°; N-[β-2-chlorostyryl], reddish brown
leaflets, m. 182-3° (from C6H6). Similarly formed were the
following 4-phenacylidene-1, 4-dihydropyridines: N-PhCH(OH)CH2, yellow
leaflets, decompose 227-8°; N-[B-4-chlorostyryl], nacreous,
orange leaflets, m. 230° (decomposition); N-(β-styryl), orange
leaflets, m. 208-9° (sintering 188°);
N-[β-2-chlorostyryl), reddish orange hexagons, m. 212°. The
following 1,4-dihydropyridines, were also formed using air and NaOH in
MeOH: 90% N-(β-styry1)-4-(1-pheny1-3-methy1-5-pyrazolon-4-ylidene),
red slender leaflets, m. 239-40° and 43%
N-(β2-chlorostyry1)-4-(2-cyclohexanonylidene), yellowish brown
leaflets, m. 192-3°. Nicotinamide MeBr salt (2.17 g.) (VIII), 3
cc. BzMe, 0.8 g. IIa, and 60 cc. MeOH under N with 2 cc. 10N NaOH gave 1
g. N-methyl-4-phenacylidene-1, 4-dihydronicotinamide (IX), yellow leaflets,
m. 278-9° (decomposition), which with HBr at 100° formed
2-methyl-5,8-dihydro-5-phenyl-8-oxo-2,7-naphthyridinium bromide, yellow
prisms, decompose 299-300°. VIII with 4-MeOC6H4Ac gave 35.2% 4-MeO
derivative of IX, brownish yellow, nacreous leaflets, decompose 277-8°;
HBr salt-H2O, vellow needles, m. 278-9° (decomposition).
N-(Diphenylmethyl)-4-(1-phenyl-3-methyl-5-pyrazolon-4-ylidene)-1,4-
dihydropyridine, yellow, prisms, m. 238-9°. IVc (0.882 g.) in 50
cc. EtOH with 0.2 g. MgO was shaken at 20° with 50 mg. Pt black and
hydrogenated. After filtration, and washing the residue with EtOH, the
evaporated filtrates gave an oil which with 5 cc. N HClO4 gave 1.15 g.
N-(2,6-dichlorobenzyl)-4-acetonylpiperidine-HClO4, colorless, m.
167-8° (from Me2CO). 39 references.
100964-61-2P, Malononitrile,
[1-(2,6-dichlorobenzyl)-4(1H)-pyridylidene]-
RL: PREP (Preparation)
   (preparation of)
100964-61-2 CAPLUS
Propanedinitrile, 2-[1-[(2,6-dichlorophenyl)methyl]-4(1H)-pyridinylidene]-
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RN

CN

(CA INDEX NAME)

OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)

L5 ANSWER 46 OF 46 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1954:39184 CAPLUS

DOCUMENT NUMBER: 48:39184

ORIGINAL REFERENCE NO.: 48:7011g-i,7012a

TITLE: Reactions of quinolinium compounds with malononitrile

and ethyl cyanoacetate

AUTHOR(S): Leonard, Nelson J.; Foster, Robert L. CORPORATE SOURCE: Univ. of Illinois, Urbana

SOURCE: Journal of the American Chemical Society (1952

), 74, 2110-11

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

AB cf. C.A. 46, 3055b. The structures erroneously assigned by Kaufmann and

Vonderwahl (C.A. 6, 2610) to condensation products derived from 1-methylquinolinium iodide (I) have been corrected. I, m. 146°

(33.6 g.), 3.3 g. CH2(CN)2 (II), and 100 cc. absolute EtCH (ice bath), treated with 2.3 g. Na in 50 cc. absolute EtCH, and the mixture stirred 3 hrs. and let stand overnight yielded 1.1 g. 1-methyl-4-dicyanomethylene)-1.4-

dihydroquinoline (III), m. 291.5-2.5°.

1-Methyl-4-chloroquinolinium iodide, m. 204-6° (1.3 g.), 0.3 g. II,

and 75 cc. absolute EtOH treated with 0.1 g. Na in 50 cc. absolute EtOH, and

the mixture stirred 8 hrs. yielded 100% III, m. 291.5-2.5°.

1,2-Dimethylquinolinium iodide (IV), m. 195-6° (14.2 g.), 3.3 g.

II, and 100 cc. absolute EtOH treated with 1.2 g. Na in 50 cc. absolute EtOH,

and

the mixture stirred 4 hrs. and let stand 4 hrs. at 25° yielded 3.8 g. 1,2-dimethyl-4-(dicyanomethylene)-1,4-dihydroguinoline, m.

267.5-68°. I and NCCH2CO2Et (V) yielded 23%

1-methyl-4-(carbethoxycyanomethylene)-1,4-dihydroguinoline m.

181.5-2.5°. IV and V gave 1,2-dimethyl-4-

(carbethoxycyanomethylene)-1,4-dihydroquinoline, m. 172.5-3.5°. I

did not yield any isolatable product with CH2(CO2Et)2, MeCN, or PhCH2CO2Et; with AcCH2CO2Et it did not give the product described by K.

IT 16344-72-2P
RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation)

(Reactions of quinolinium compounds with malononitrile and ethyl cvanoacetate)

RN 16344-72-2 CAPLUS

CN Propanedinitrile, 2-(1-methyl-4(1H)-pyridinylidene)- (CA INDEX NAME)

OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

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